Comment on the Specific Heat of a Bose Gas Confined to a Thin-Film Geometry*

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(Received 21 February 1973; revised manuscript received 12 June 1973)

Our previous evaluation of the specific heat of an ideal Bose gas confined to a thin-film geometry is extended to second order in $(\bar{l}/D)$, where $\bar{l}$ is the mean interparticle distance. Explicit expressions, involving a dimensionless parameter y, are obtained both for the specific heat of the system and for the temperature at which the specific heat is maximum. Occurrence of the parameter y, which is a measure of the chemical potential of the system in terms of the spacing of the single-particle energy levels, enables us to cast our expression for the specific heat of the system into a form consistent with the scaling theory of Fisher and Barber. Our results for the specific-heat maximum, as a function of $(D/\bar{l})$, are a considerable improvement over the first-order ones reported earlier, and have come remarkably close to the ones obtained numerically by Goble and Trainor.

I. INTRODUCTION

In a previous paper[1] (hereafter denoted as I) the phenomenon of Bose-Einstein condensation in thin films was investigated analytically so as to determine the rigorous asymptotic behavior of the specific heat of the system in the "critical region." In that investigation, summations over states appearing in the various expressions pertaining to the system were evaluated without having recourse to the customary procedure (of converting summations into integrations) which is liable to serious inaccuracies when applied to a finite system. Using analytical techniques, asymptotic expressions for $T_{\max}(D)$ and $C_{\max}(D)$, pertaining to the specific-heat maximum, were derived to *first* order in $(\bar{l}/D)$, where $\bar{l}$ is the mean interparticle distance and D is the film thickness. These results turned out to be in good qualitative agreement with the corresponding numerical ones obtained by Goble and Trainor.[2] Quantitatively, however, the agreement was not very satisfactory. In particular, the value D^* of the film thickness at which the specific heat of the system, under Dirichlet boundary conditions ($\psi_S=0$), possesses an *absolute* maximum was found to be $31.1\bar{l}$, which is rather large in comparison with the value $(17.5\pm1.5)\bar{l}$ obtained by Goble and Trainor. Similarly, the value of the absolute maximum, in units of Nk, was found to be 1.9583, which is rather small in comparison with the corresponding value of Goble and Trainor, viz., 1.970 ± 0.002.

We have now extended the analysis of I to *second* order in $(\bar{l}/D)$ and have obtained results which are in excellent quantitative agreement with the corresponding ones of Goble and Trainor. For instance, the new values of D^* and $C_{\max}(D^*)$ turn out to be $19.4\bar{l}$ and $1.9688Nk$ which are remarkably close to the values of Goble and Trainor. This indicates that the convergence of our asymptotic expansions is quite rapid.

Recently, Barber and Fisher[3] have investigated the same problem using different mathematical techniques. Their first-order results for $T_{\max}(D)$ and $C_{\max}(D)$ are in complete agreement with the ones reported in I. Their higher-order results, which are essentially second order, are in good accord with the ones being reported here; see footnote to Table I. Barber and Fisher have also shown that in the "critical region," viz., $T\simeq T_{\max}(D)$ their results are in agreement with the scaling theory for finite-size effects developed by them earlier.[4] We find that our formulation is not only consistent with the scaling theory but also elucidates the underlying reason for this, i.e., the occurrence of a dimensionless parameter y which appeared naturally in I and which determines, in the manner of a *law of corresponding states*, the asymptotic behavior of the given system in the "critical region." The physical significance of the parameter y is examined, in the hope that it may lead to a possible generalization of the scaling hypothesis to systems with different geometries and to systems with interparticle interactions.

II. SUMMARY OF THE ANALYSIS

As shown in I, the specific heat of a Bose-Einstein system of noninteracting particles, with mean occupation numbers $\langle n_i\rangle$ for the single-particle energy levels ϵ_i, is given by

$$C_V=k(G_2-G_1^2/G_0)\,, \tag{1}$$

where

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

TABLE I. Data corresponding to the *absolute* specific-heat maximum of a Bose-Einstein film under Dirichlet boundary conditions.

	First-order results (Ref. 1)	Second-order results (present work)	Numerical results (Ref. 2)
$D^*/\bar{l}$	31.1	19.4 [a]	17.5±1.5
$C_{max}(D^*)/Nk$	1.9583	1.9688 [a]	1.970±0.002

[a] Corresponding values obtained by Barber and Fisher (Ref. 3) are $(D^*/\bar{l}) \simeq 20$ and $C_{max}(D^*)/Nk \simeq 1.9675$, respectively.

$$Z_s = \sum_i \left(\frac{\epsilon_i}{kT}\right)^s \langle n_i \rangle, \quad \alpha = -(\mu/kT), \tag{3}$$

μ being the chemical potential of the system. These 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 constitutes the central problem of our approach.

Since the publication of I, we have developed a new method of evaluating the functions Z_s for a system in the form of an infinite slab (of thickness D). This method not only obviates the contour integration technique of Krueger[5] but also affords a straightforward, yet rigorous, generalization to systems of other shapes.[6] For the infinite slab, we obtain

$$Z_s = \frac{V}{\lambda^3}\left(\frac{\Gamma(s+\frac{3}{2})}{\Gamma(\frac{3}{2})} g_{s+3/2}(\alpha) + \tfrac{1}{2}\Theta(\lambda/D)\Gamma(s+1)g_{s+1}(\alpha) + \frac{2}{(1+\Theta^2)}(\lambda/D)(-\alpha)^s g_1(2y)\right), \tag{4}$$

where $\Gamma(x)$ denotes the Γ function of x while $g_n(\delta)$ are the familiar Bose-Einstein functions[7]

$$g_n(\delta) = \frac{1}{\Gamma(n)} \int_0^\infty \frac{x^{n-1}\,dx}{e^{x+\delta}-1}. \tag{5}$$

In addition, $\lambda[=h/(2\pi MkT)^{1/2}]$ denotes the mean thermal wavelength of the particles, while $\Theta=-1$, $+1$, or 0 according as the boundary conditions employed are Dirichlet, Neumann, or periodic. Finally, the parameter y is defined by

$$y = (1+\Theta^2)\pi^{1/2}(D/\lambda)\alpha^{1/2}. \tag{6}$$

Noting that $Z_0 \equiv N$, we have

$$N(\alpha, T, D) = \frac{V}{\lambda^3}\left(g_{3/2}(\alpha) + \frac{2}{(1+\Theta^2)}(\lambda/D) \times g_1(2y) + \tfrac{1}{2}\Theta(\lambda/D)g_1(\alpha)\right) \tag{7}$$

which, to *second* order in (λ/D), may be written

$$\left(\frac{\lambda}{\bar{l}}\right)^3 + \left(\frac{\lambda}{D}\right)\Lambda\left(y, \frac{D}{\lambda}\right) + \left(\frac{\lambda}{D}\right)^2\left(\frac{\zeta(\frac{1}{2})y^2}{\pi(1+\Theta^2)^2}\right) = \zeta(\tfrac{3}{2}), \tag{8}$$

where

$$\Lambda\left(y, \frac{D}{\lambda}\right) = \frac{2}{(1+\Theta^2)}\ln(2\sinh y) - \Theta\ln\left(\frac{(1+\Theta^2)\pi^{1/2}}{y}\frac{D}{\lambda}\right). \tag{9}$$

To the same order in (λ/D), the specific heat of the system is given by

$$C_V/Nk = (\bar{l}/\lambda)^3[\tfrac{15}{4}\zeta(\tfrac{5}{2}) + a_1(\lambda/D) + a_2(\lambda/D)^2], \tag{10}$$

where

$$a_1 = \Theta\zeta(2) - \tfrac{9}{4}\frac{[\zeta(\frac{3}{2})]^2}{\pi(1+\Theta^2)}M(y), \tag{11}$$

$$a_2 = -\tfrac{15}{4}\frac{\zeta(\frac{3}{2})y^2}{\pi(1+\Theta^2)^2} + \frac{3\zeta(\frac{3}{2})M(y)}{\pi(1+\Theta^2)} \times\left(\tfrac{3}{4}\frac{\zeta(\frac{3}{2})\zeta(\frac{1}{2})}{\pi(1+\Theta^2)}M(y) + \Lambda(y, D/\lambda) + \frac{y}{(1+\Theta^2)}\coth y\right), \tag{12}$$

and

$$M(y) = \left(\frac{\coth y}{y} + \frac{1}{2}\frac{\Theta(1+\Theta^2)}{y^2}\right)^{-1}.$$

Using (8) and (9), expression (10) for (C_V/Nk) can be expressed in terms of $(\bar{l}/D)$ rather than (λ/D). In the vicinity of $T_0(\infty)$, which denotes the critical point of the bulk system, we obtain

$$C_V/Nk = \tfrac{15}{4}[\zeta(\tfrac{5}{2})/\zeta(\tfrac{3}{2})] + b_1(\bar{l}/D) + b_2(\bar{l}/D)^2, \tag{13}$$

where b_1 and b_2 are somewhat complicated functions of y and depend implicitly on $(\bar{l}/D)$ as well.

The value of y for which the specific heat of the system is maximum now turns out to be of the form

$$y_{max} = y_0 + (\bar{l}/D)[\gamma\ln(D/\bar{l}) + \delta], \tag{14}$$

where y_0 is the value of y_{max} obtained in I. It will be noted that the existence of a *unique* value of y_0, irrespective of the actual value of D, is closely related to the applicability of the scaling theory for finite-size effects to the system under study!

III. RESULTS AND DISCUSSION

(i) In the case of periodic boundary conditions ($\Theta=0$), we find

$$y_{max} = 0.85396 + 0.45102\,(\bar{l}/D), \tag{15}$$

whence

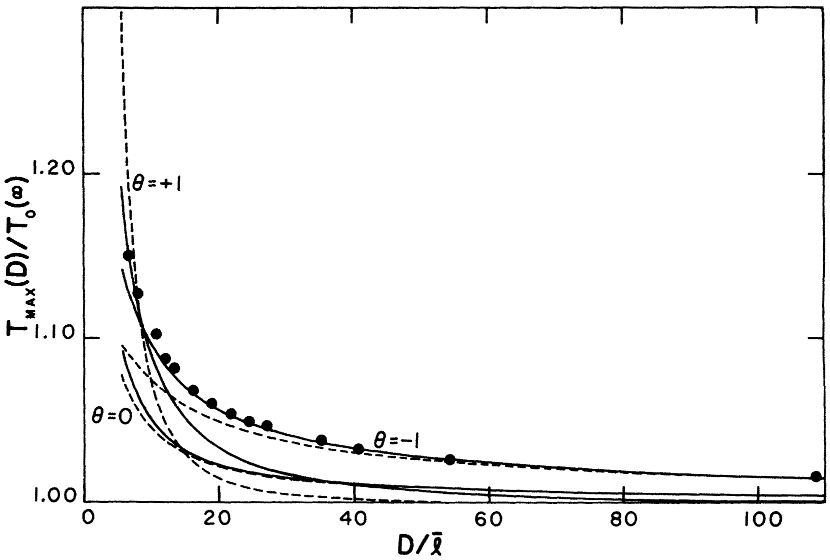

FIG. 1. Temperature $T_{max}(D)$ at which the specific heat of an infinite slab of thickness D is maximum: first-order results, dashed line; second-order results, solid line. Numerical results of Goble and Trainor (for $\Theta = -1$) are shown by closed circles.

$$T_{max}(D)/T_0(\infty) = 1 + 0.45971(\bar{l}/D) + 0.45182(\bar{l}/D)^2 \tag{16}$$

and

$$C_{max}(D)/Nk = 1.92567 - 0.19734(\bar{l}/D) - 0.07056(\bar{l}/D)^2 . \tag{17}$$

These results are plotted in Figs. 1 and 2.

(ii) In the case of Dirichlet boundary conditions ($\Theta = -1$), we find that[8]

$$y_{max} = i\{2.68718 + 0.69078(\bar{l}/D) - 0.94012(\bar{l}/D)\ln(D/\bar{l})\}, \tag{18}$$

whence

$$T_{max}(D)/T_0(\infty) = 1 + 0.35147(\bar{l}/D)[\ln(D/\bar{l}) - 0.17333] + 0.09265(\bar{l}/D)^2 \times\{[\ln(D/\bar{l})]^2 + 8.94802\ln(D/\bar{l}) - 2.04080\} \tag{19}$$

and

$$C_{max}(D)/Nk = 1.92567 + 1.01522(\bar{l}/D)[\ln(D/\bar{l}) - 2.43721] + 0.35682(\bar{l}/D)^2 \times\{[\ln(D/\bar{l})]^2 + 0.70878\ln(D/\bar{l}) + 5.40997\}. \tag{20}$$

These results are also plotted in Figs. 1 and 2

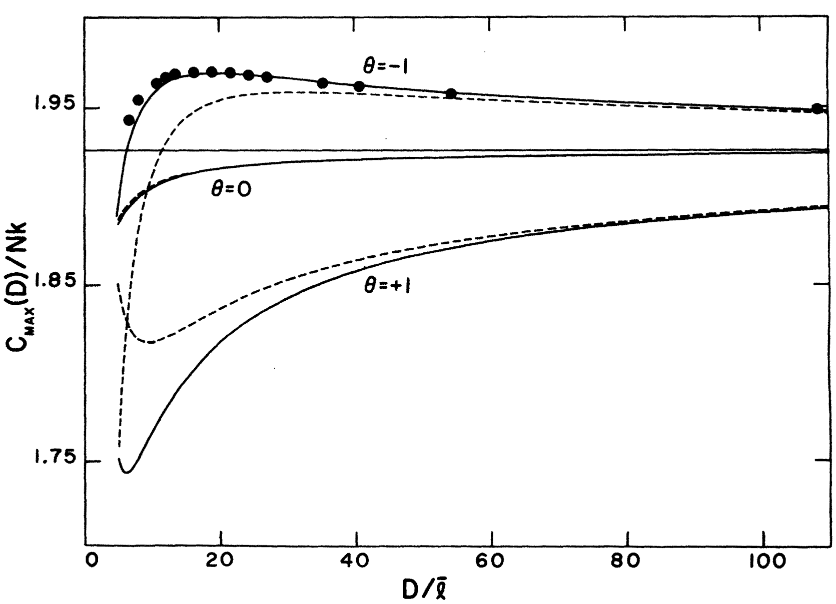

FIG. 2. Height $C_{max}(D)$ of the specific-heat maximum: first-order results, dashed line; second-order results, solid line. Numerical results of Goble and Trainor (for $\Theta = -1$) are shown by closed circles while the horizontal line corresponds to the bulk value $C_0(\infty)$.

and are in excellent agreement with the numerical results of Goble and Trainor.[2]

A better indication of the accuracy of our analysis is obtained by examining the value, $(D^*/\bar{l})$, of $(D/\bar{l})$ at which the specific heat of the system is at an absolute maximum; one may also look at the corresponding value, $C_{max}(D^*)/Nk$, of $C_{max}(D)/Nk$. Table I contains results for these numbers as obtained in I, the second-order results as obtained in the present investigation, and the Goble-Trainor results obtained numerically. Corresponding results of Barber and Fisher are also given.

(iii) In the case of Neumann boundary conditions $(\Theta=+1)$, we find that

$$y_{max}=4.40186+43.95623(\bar{l}/D)-19.84056(\bar{l}/D)\ln(D/\bar{l}), \tag{21}$$

whence

$$T_{max}(D)/T_0(\infty)=1-0.35147(\bar{l}/D)[\ln(D/\bar{l})-4.93831]+0.09265(\bar{l}/D)^2\times\{[\ln(D/\bar{l})]^2-101.59910\times\ln(D/\bar{l})+214.01556\} \tag{22}$$

and

$$C_{max}(D)/Nk=1.92567-1.01522(\bar{l}/D)\times[\ln(D/\bar{l})-1.24145]+0.35682(\bar{l}/D)^2\times\{[\ln(D/\bar{l})]^2-14.78192\times\ln(D/\bar{l})+14.22426\}. \tag{23}$$

These results are also included in Figs. 1 and 2. The "spurious" minimum in the value of $C_{max}(D)/Nk$, first encountered in I, is now shifted to a lower value of $(D/\bar{l})$, as was indeed expected. Of course, as remarked in I, the validity of asymptotic analysis at such low values of $(D/\bar{l})$ is rather questionable.

To show that our formulation is consistent with the scaling theory for finite-size effects,[4] we first of all note that the scaling hypothesis is expected to apply if, and only if,

$$(D/\bar{l})\gg 1$$

and

$$[T-T_0(\infty)]/T_0(\infty)\ll 1. \tag{24}$$

These conditions lead one to consider *only first-order results in* $(\bar{l}/D)$. We then expect that the specific heat $C_V(T)$, in the "critical region," is governed by the variable

$$z=(D/\bar{l})\dot{t}, \tag{25}$$

where $\dot{t}$ represents the shifted temperature deviation as defined by

$$\dot{t}=[T-T_{max}(D)]/T_0(\infty). \tag{26}$$

Conditions (24) imply that $\dot{t}$ is also much less than unity. Now, it can be shown that

$$z=(D/\bar{l})\dot{t}\simeq\tfrac{2}{3}[\zeta(\tfrac{3}{2})]^{-2/3}\left[\Lambda\left(y,\frac{D}{\lambda_0(\infty)}\right)-\Lambda\left(y_0,\frac{D}{\lambda_0(\infty)}\right)\right]=\tfrac{2}{3}[\zeta(\tfrac{3}{2})]^{-2/3}\left[\frac{2}{(1+\Theta^2)}ln\left(\frac{\sinh y}{\sinh y_0}\right)+\Theta\ln(y/y_0)\right]. \tag{27}$$

Clearly, the scaling variable z is *a function of* y *alone;* in particular, for $y=y_0$, $z=0$.[9] In turn, it follows that y is a function of z alone (though an explicit relationship to express this dependence can be written only for $\Theta=0$). We may, therefore, expect that the specific heat of the system in the "critical region" is governed by the parameter y. This is indeed true, for we can write

$$\frac{C_V(T,D)}{Nk}\simeq\frac{C_V(T_{max},D)}{Nk}+(\bar{l}/D)\times\left(\frac{45}{8}[\zeta(\tfrac{3}{2})]^{-1}\zeta(\tfrac{5}{2})z(y)-\frac{9}{4}\frac{[\zeta(\tfrac{3}{2})]^{4/3}}{\pi(1+\Theta^2)}\times[M(y)-M(y_0)]\right). \tag{28}$$

We also find that our scaling function, i.e., the coefficient of $(\bar{l}/D)$ in (28), is equivalent to the corresponding function of Barber and Fisher[3] for each of the boundary conditons considered by them, viz., $\Theta=0$ and $\Theta=-1$.

Further insight into the physical significance of the parameter y is gained by observing that

$$y=(1+\Theta^2)\pi^{1/2}(D/\lambda)\alpha^{1/2}=\pi(-\mu/\Delta)^{1/2}, \tag{29}$$

where $\Delta[=\hbar^2/(MD^2)]$ is a measure of the discreteness of the (low-lying) energy levels of the system arising from the finiteness of one of its dimensions. The parameter y^2, therefore, represents the chemical potential of the system "reduced in terms of the energy parameter Δ." It thus appears that, in the system under study, as we approach temperatures where the conventional parameter $\alpha[=-(\mu/kT)]$ becomes very small, $0(\lambda^2/D^2)$ instead of $0(1)$, the thermodynamics of the system is governed by the parameter y^2. It seems plausible that this result, although derived here for an ideal Bose-Einstein film, may be valid for interacting systems as well. If so, the validity of the scaling hypothesis for such systems would also be guaranteed.

ACKNOWLEDGMENTS

We wish to thank Professor Michael E. Fisher and Dr. Michael N. Barber for sending us a copy of their manuscript prior to publication and for other helpful correspondence on this subject.

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*Work supported in part by the National Research Council of Canada.

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[8] An imaginary y_{max} means that the corresponding value, α_{max}, of α is negative; see Eq. (6). This point has already been discussed in I.

[9] It will be noted that, over the entire region of interest, y and z are of the order of unity.