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Comments and Addenda

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Effect of boundary conditions on finite Bose-Einstein assemblies*

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The recent observation by Hasan and Goble of a discrepancy between their numerical results on the specific heat of an ideal Bose gas confined to a thin-film geometry and the earlier analytic calculations of Pathria employing Neumann boundary conditions is shown to be unjustified. In those cases where a true comparison is possible, e.g., under Dirichlet or periodic boundary conditions, the observed deviations turn out to be insignificant if one uses the more recent second-order calculations of Greenspoon and Pathria rather than the original first-order ones of Pathria. For comparison under Neumann boundary conditions, fresh numerical calculations are required. We also present here second-order analytic calculations of the specific heat of this system (i) under mixed boundary conditions (Dirichlet on one wall, Neumann on the other) and (ii) under antiperiodic boundary conditions, and compare them with the relevant numerical calculations of Hasan and Goble.

I. INTRODUCTION

In a recent paper Hasan and Goble[1] have considered the effect of boundary conditions on the specific heat of a finite Bose-Einstein assembly. Their observation of a discrepancy between some of their numerical results and the asymptotic analytic calculations of Pathria[2] (hereafter referred to as I) for the specific heat of an ideal Bose film under Neumann boundary conditions is unjustified, because the energy spectrum employed by Hasan and Goble is inappropriate to these boundary conditions. In fact, their spectrum corresponds to mixed boundary conditions (Dirichlet on one wall, Neumann on the other),[3] for which analytic calculations have so far been lacking. This motivated us to investigate analytically the specific heat of a thin Bose film under the aforementioned boundary conditions. It turns out that with minor adjustments the results obtained for this case become applicable to antiperiodic boundary conditions[4] as well.

Deviations between numerical and analytic calculations, under Dirichlet boundary conditions, are indeed significant if one employs the first-order analytic results of I; however, they become insignificant when comparison is made with the second-order results of Greenspoon and Pathria[5] (hereafter referred to as II). This, in fact, had already been demonstrated in II, but Hasan and Goble were apparently unaware of that paper at the time of writing theirs.

II. ANALYTIC RESULTS AND DISCUSSION

We consider an ideal Bose gas confined to a thin-film geometry ($L\times L\times D$, $L\to\infty$) under the following sets of boundary conditions for the single-particle wave functions ψ:

(i) *Mixed boundary conditions,* so that

$$\begin{aligned}&\psi_{x=0}=\psi_{y=0}=\psi_{z=0}=0\,;\\&(\partial\psi/\partial\hat{n})_{x=L}=(\partial\psi/\partial\hat{n})_{y=L}=(\partial\psi/\partial\hat{n})_{z=D}=0\,.\end{aligned}\tag{1}$$

(ii) *Antiperiodic boundary conditions,* so that

$$\psi_{x+L,\,y,\,z}=\psi_{x,\,y+L,\,z}=\psi_{x,\,y,\,z+D}=-\psi_{x,\,y,\,z}\,.\tag{2}$$

The corresponding energy spectra turn out to be

$$\text{(i)}\quad \epsilon_{lmn}=\frac{\pi^2\hbar^2}{2M}\left(\frac{(l+\frac{1}{2})^2+(m+\frac{1}{2})^2}{L^2}+\frac{(n+\frac{1}{2})^2}{D^2}\right),\qquad l,m,n=0,1,2,\ldots\tag{3}$$

$$\text{(ii)}\quad \epsilon_{lmn}=\frac{2\pi^2\hbar^2}{M}\left(\frac{(l+\frac{1}{2})^2+(m+\frac{1}{2})^2}{L^2}+\frac{(n+\frac{1}{2})^2}{D^2}\right),\qquad l,m,n=0,\pm1,\pm2,\ldots.\tag{4}$$

In their numerical work, Hasan and Goble have employed energy spectrum (3), which pertains to mixed boundary conditions and *not* to Neumann boundary conditions. The spectrum pertaining to Neumann boundary conditions is instead given by

$$\epsilon_{lmn}=\frac{\pi^2\hbar^2}{2M}\left(\frac{l^2+m^2}{L^2}+\frac{n^2}{D^2}\right),\quad l,m,n=0,1,2,\ldots\,; \tag{5}$$

see Eq. (14) of I. A comparison of the numerical results obtained by Hasan and Goble using energy spectrum (3) with the analytic calculations based on energy spectrum (5) is clearly unjustified. For a proper comparison with the analytic results of I, or better II, fresh numerical calculations using energy spectrum (5) are required.

For studying the specific heat of the system, with energy spectra (3) and (4), we follow the method developed recently by Greenspoon and Pathria[6] (hereafter referred to as III). Integrating over the x and y dimensions of the film, we obtain for the total number of particles in the system

$$N=\frac{L^2}{\lambda^2}\sum_{j=1}^{\infty}\frac{e^{-j\alpha}}{j}\sum_{n}e^{-j(n+1/2)^2w}, \tag{6}$$

where $\alpha=-\mu/kT$, μ being the chemical potential,

$$w=\eta^2\pi(\lambda/D)^2,\quad \lambda=\hbar(2\pi/MkT)^{1/2}, \tag{7}$$

while $\eta=\frac{1}{2}$ for the mixed boundary conditions and 1 for the antiperiodic.

Now, for *both* the boundary conditions, the sum over n in (6) may be written

$$\sum_n=\eta e^{-(1/4)jw}\sum_{n=-\infty}^{\infty}[e^{-jwn^2}\cosh(jwn)-e^{-jwn^2}\sinh(jwn)]. \tag{8}$$

While the second part vanishes identically, the first part can be simplified by using Poisson's summation formula and taking the appropriate Fourier transform.[7] Equation (8) thereby becomes

$$\sum_n=\eta\left(\frac{\pi}{jw}\right)^{1/2}\left(1+2\sum_{q=1}^{\infty}(-1)^q e^{-\pi^2q^2/jw}\right). \tag{9}$$

Substituting (9) into (6) and converting the sum over j into an integral, as in III, we finally obtain

$$N=(V/\lambda^3)[g_{3/2}(\alpha)+2\eta(\lambda/D)h_1(2y)], \tag{10}$$

where $g_n(\alpha)$ are the familiar Bose-Einstein functions,[8] while

$$h_1(2y)=\sum_{q=1}^{\infty}(-1)^q\frac{e^{-2qy}}{q}=y-\ln(2\cosh y) \tag{11}$$

and

$$y=\frac{\pi^{1/2}\alpha^{1/2}}{\eta}\frac{D}{\lambda}=\frac{1}{2\eta}\frac{D}{\xi}, \tag{12}$$

ξ $[=\lambda/(2\pi^{1/2}\alpha^{1/2})]$ being the correlation length for the bulk system. The physical significance of the *thermogeometric parameter* y, in relation to the scaling theory for finite-size effects,[4] has been elucidated in II and III.

In passing we note the absence of a $g_1(\alpha)$ term in (10); cf. Eq. (22) of I. Accordingly, we do not expect to obtain logarithmic terms in the final expressions, such as (17)–(19); cf. the corresponding expressions in I and II. This is closely related to the fact that, under the boundary conditions employed here, the density of states of the system does not contain a surface correction.[9] The absence of such a correction when the opposite walls of the box satisfy opposite boundary conditions (Dirichlet on one, Neumann on the other) has been pointed out previously by Pathria.[3]

The specific heat and its temperature derivatives are ultimately derived from the functions

$$Z_s=\sum_i\left(\frac{\epsilon_i}{kT}\right)^s\langle n_i\rangle. \tag{13}$$

As shown in III, Z_s can be obtained straightforwardly from the expression for N, which is, in fact, Z_0. Following procedures similar to those in I and II, we find that, to second order in $\bar{l}/D$, where $\bar{l}$ is the mean interparticle distance in the system, the specific heat of the system is given by

$$C_V(D)/Nk=\tfrac{15}{4}\zeta(\tfrac{5}{2})/\zeta(\tfrac{3}{2})+b_1(\bar{l}/D)+b_2(\bar{l}/D)^2, \tag{14}$$

where

$$b_1=\eta[\zeta(\tfrac{3}{2})]^{-5/3}\{\tfrac{15}{2}\zeta(\tfrac{5}{2})\ln(2\cosh y)-(9/4\pi)[\zeta(\tfrac{3}{2})]^3y\coth y\} \tag{15}$$

and

$$b_2=\eta^2[\zeta(\tfrac{3}{2})]^{-7/3}\left(\frac{3[\zeta(\frac{3}{2})]^3}{\pi}y\coth y\ln(2\cosh y)+\frac{9y^2}{4\pi^2}[\zeta(\tfrac{3}{2})]^4\zeta(\tfrac{1}{2})\coth^2y+10\zeta(\tfrac{5}{2})[\ln(2\cosh y)]^2-\frac{3}{4\pi}[\zeta(\tfrac{3}{2})]^3y^2+\frac{15}{4\pi}\zeta(\tfrac{5}{2})\zeta(\tfrac{3}{2})\zeta(\tfrac{1}{2})\right). \tag{16}$$

Equating $(\partial C_V/\partial T)_{N,D}$ to zero, we find that the specific-heat maximum corresponds to

$$y_{\max}=1.08639+0.23471\eta(\bar{l}/D). \tag{17}$$

We note that in the limit $D\gg\bar{l}$, where scaling theory applies, the two cases under study are governed by the same value of $y_{\max}$.

To the same order in $(\bar{l}/D)$, the temperature cor-

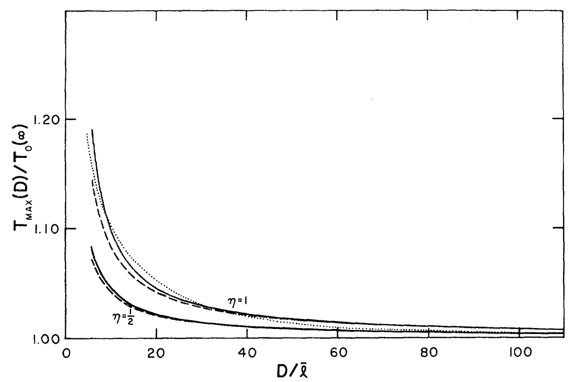

FIG. 1. Temperature $T_{max}(D)$ at which the specific heat of an infinite slab of thickness D is maximum. First-order results: dashed line; second-order results: solid line. The dotted line represents the numerical results of Hasan and Goble for the case $\eta=\frac{1}{2}$.

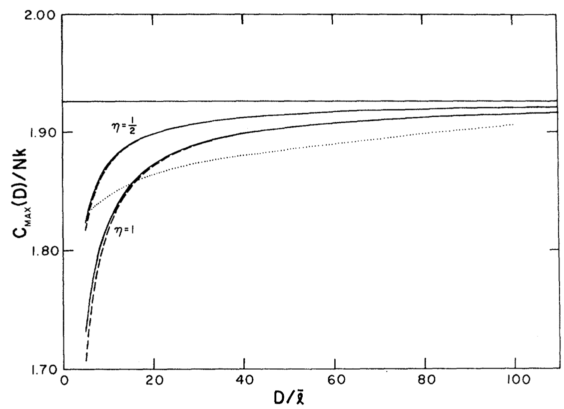

FIG. 2. Height $C_{max}(D)$ of the specific-heat maximum. First-order results: dashed line; second-order results: solid line. The dotted line represents the numerical results of Hasan and Goble for the case $\eta=\frac{1}{2}$, while the horizontal line corresponds to the bulk value $C_0(\infty)$.

responding to the specific-heat maximum turns out to be

$$T_{max}(D)/T_0(\infty)=1+0.839\,46\eta(\bar{l}/D)+1.575\,49\eta^2(\bar{l}/D)^2\,. \tag{18}$$

These results are plotted in Fig. 1. For the height of the specific-heat maximum, we obtain

$$C_{max}(D)/Nk=1.925\,67-1.094\,01\eta(\bar{l}/D)+0.611\,55\eta^2(\bar{l}/D)^2\,. \tag{19}$$

These results are plotted in Fig. 2.

Our analytic results for mixed boundary conditions ($\eta=\frac{1}{2}$) are in very poor agreement with the numerical ones of Hasan and Goble, even though they are based on the same energy spectrum (3). In view of the excellent agreement between our analytic and their numerical results for Dirichlet and periodic boundary conditions, see II, the present discrepancy is indeed baffling. At first we thought that this may have been due to a possible error in the Jacobi transformation employed by Hasan and Goble for their numerical work; note that, instead of what we have on the right-hand side of (9), they have

$$\frac{1}{2}\left(\frac{\pi}{jw}\right)^{1/2}e^{jw/4}\left(1+\sum_{q=1}^{\infty}(-1)^q e^{-\pi^2q^2/jw}\right).$$

However, in a private communication, Professor Goble has informed us that the Jacobi transformation actually employed in their work was indeed the correct one, and not the one that inadvertently appeared in their paper; consequently, the source of error in the numerical computation must lie somewhere else.

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[1]Z. R. Hasan and D. F. Goble, Phys. Rev. A 10, 618 (1974).

[2]R. K. Pathria, Phys. Rev. A 5, 1451 (1972), referred to as I.

[3]R. K. Pathria, Nuovo Cimento Suppl. 4, 276 (1966).

[4]M. E. Fisher and M. N. Barber, Phys. Rev. Lett. 28, 1516 (1972).

[5]S. Greenspoon and R. K. Pathria, Phys. Rev. A 8, 2657 (1973), referred to as II.

[6]S. Greenspoon and R. K. Pathria, Phys. Rev. A 9, 2103 (1974), referred to as III.

[7]*Tables of Integral Transforms*, edited by A. Erdelyi (McGraw-Hill, New York, 1954), Vol. 1, p. 35.

[8]R. K. Pathria, *Statistical Mechanics* (Pergamon, New York, 1972), p. 177.

[9]R. K. Pathria, Phys. Lett. 35A, 351 (1971).