

Bose-Einstein condensation in arbitrarily shaped cavities

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We discuss the phenomenon of Bose-Einstein condensation of an ideal nonrelativistic Bose gas in an arbitrarily shaped cavity. The influence of the finite extension of the cavity on all thermodynamical quantities, especially on the critical temperature of the system, is considered. We use two main methods that are shown to be equivalent. The first deals with the partition function as a sum over energy levels and uses a Mellin-Barnes integral representation to extract an asymptotic formula. The second method converts the sum over the energy levels to an integral with a suitable density of states factor obtained from spectral analysis. The application to some simple cavities is discussed. [S1063-651X(99)03101-3]

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I. INTRODUCTION

It is now well over 70 years since the phenomenon referred to as Bose-Einstein condensation (BEC) was first predicted [1,2]. Until recently the best experimental evidence that BEC could occur in a real physical system was liquid helium, as suggested originally by London [3]. More recently it was suggested [4,5] that BEC could occur for excitons in certain types of nonmetallic crystals (such as CuCl, for example). There is now good evidence for this in a number of experiments [6]. However, the most exciting experimental evidence for BEC has come from the observations of very cold alkali gases. BEC has now been observed to occur in gases of rubidium [7], lithium [8], and sodium [9]. In these experiments BEC has been realized in magnetic traps and laser traps, in small volumes far away from the infinite volume limit. Although nowadays a few million particles remain in the trap, in these early experiments only up to 2000 particles remained there so that it was by no means clear if calculations done in the thermodynamical limit are an accurate treatment when considering this experimental situation. (For a more detailed analysis of this see Refs. [10–15].) This motivates us to consider the related problem of the quantum statistics of a finite number of particles in an arbitrarily shaped cavity.

When thinking about quantum statistics in finite volumes there appears an immediate difference to the thermodynamic limit. Quantum particles confined to a finite volume of arbitrary size inevitably have a nonzero kinetic energy, hence they must exert some pressure. Taking μm -sized cavities and the parameters typical for liquid helium it can be seen that the zero-point pressure is of measurable magnitude [16]. But not only the pressure but also all other thermodynamical quantities may deviate substantially from the results obtained in the thermodynamical limit once the volume and the par-

ticle number get small enough. In this article we want to give a systematic treatment of this problem.

In doing this we are going to extend a recent careful and beautiful study of BEC in a cubic volume where the gas was supposed to fulfill Dirichlet boundary conditions at the boundary of the cavity [16]. The authors there employed an approach where the sum over the discrete spectrum was replaced by an integral with an appropriate density of states. This density was obtained by the knowledge of the energy spectrum in this example.

In this article we are going to treat an arbitrarily shaped cavity. The methods we are going to employ are the so-called heat-kernel techniques extensively used in finite temperature relativistic quantum field theory starting with the work of Dowker and Kennedy [17]. However, in these considerations the stress was more on the influence of gravitational fields on the quantum statistics (see also [18]). Recently also the influence of boundaries was considered in the context of the Casimir effect [19,20] and of BEC as symmetry breaking [21,22]. In nonrelativistic theories these techniques are, however, nearly unemployable and we want to show in the present article that they also can be used here in a very effective way.

The plan of the paper is as follows. First we develop the quantum statistics of N noninteracting bosons in a finite cavity of arbitrary shape. We will exemplify the use of heat-kernel techniques and of the Mellin-Barnes integral representation for the calculation of the partition function. We will explicitly show what influence the boundary and its shape have on all thermodynamical quantities, especially on the critical temperature at which BEC occurs. In Sec. III we describe an alternative approach where sums are converted into ordinary integrals with an appropriate density of states factor. We will show that the density of states is determined by the heat-kernel coefficients of the associated Schrödinger operator. The next section is devoted to the discussion of some specific examples like the rectangular box and the spherical cavity with various boundary conditions. In the final section we present a short summary of our main results.

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II. QUANTUM STATISTICS OF A FREE BOSE GAS IN A d -DIMENSIONAL FINITE CAVITY

Let us consider a system of N noninteracting bosons in a finite cavity \mathcal{M} with boundary $\partial\mathcal{M}$ and with single-particle state energies E_N determined by the Schrödinger equation

$$-\frac{\hbar^2}{2m}\Delta\phi_N(x)=E_N\phi_N(x); \quad \phi_N|_{x\in\partial\mathcal{M}}=\dots, \quad (2.1)$$

where we do not need to fix here the boundary conditions imposed on the field because our treatment will be quite general.

In the grand canonical approach, the partition sum then reads

$$q = -\sum_N \ln(1 - ze^{-\beta E_N}), \quad (2.2)$$

with the fugacity $z = \exp(\beta\mu)$, μ being the chemical potential and $\beta = 1/(kT)$. In the discussion of BEC the ground state always plays a special role and for that reason we write

$$q = q_0 - \sum_N' \ln(1 - ze^{-\beta E_N}). \quad (2.3)$$

Here the prime indicates that the ground state is to be omitted and q_0 is the contribution of the ground state with energy E_0 and degeneracy d_0 ,

$$q_0 = -d_0 \ln(1 - ze^{-\beta E_0}). \quad (2.4)$$

For the calculation of the partition sum, Eq. (2.3), we will first expand the logarithm to obtain

$$q = q_0 + \sum_{n=1}^{\infty} \sum_N' \frac{1}{n} e^{-\beta n(E_N - \mu)}. \quad (2.5)$$

For the evaluation of this kind of expressions it is very effective to make use of the Mellin-Barnes type integral representations,

$$e^{-v} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha \Gamma(\alpha) v^{-\alpha}, \quad (2.6)$$

valid for $\text{Re } v > 0$ and $c \in \mathbb{R}$, $c > 0$. Equation (2.6) is easily proven by closing the contour to the left obtaining immediately the power series expansion of $\exp(-v)$. Using Eq. (2.6) in (2.5) we find (defining $\mu_c = E_0$)

$$\begin{aligned} q &= q_0 + \sum_{n=1}^{\infty} \frac{1}{n} e^{-n\beta(\mu_c - \mu)} \sum_N' e^{-n\beta(E_N - E_0)} \\ &= q_0 + \sum_{n=1}^{\infty} \frac{1}{n} e^{-n\beta(\mu_c - \mu)} \\ &\quad \times \sum_N' \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha \Gamma(\alpha) (\beta n)^{-\alpha} (E_N - E_0)^{-\alpha}. \end{aligned} \quad (2.7)$$

At this stage we would like to interchange the summations over N and n and the integration in order to arrive at an expression containing the ζ function associated with the Schrödinger equation (2.1),

$$\zeta(s) = \sum_N' (E_N - \mu_c)^{-s}. \quad (2.8)$$

General zeta function theory tells us that the rightmost pole of $\zeta(s)$ is located at $s = d/2$, see for example [23], followed by poles at $s = (d-1)/2, \dots, 1/2; -(2l+1)/2$, $l \in \mathbb{N}_0$. In general the rightmost pole appears at $s = d/m$ where d is the dimension of space and m is the order of the elliptic differential operator, here 2. Furthermore, we need the polylogarithm,

$$\text{Li}_n(x) = \sum_{l=1}^{\infty} \frac{x^l}{l^n}, \quad (2.9)$$

basic properties of which may be found in [24,25]. As we will see in the following, the treatment of arbitrary dimension d creates no additional complications. But it may not be of only academic interest. In this context we mention the analogies between bosons in a two-dimensional box and bosons in a one-dimensional harmonic oscillator potential analyzed in Ref. [26]. Similar analogies between higher-dimensional cavities and external potentials in dimensions $d = 1, 2, 3$ remain to be explored.

Due to the above remarks, in order that the summation and integration might be interchanged we have to impose that $\text{Re } c > d/2$ to obtain

$$q = q_0 + \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha \Gamma(\alpha) \beta^{-\alpha} \text{Li}_{1+\alpha}(e^{-\beta(\mu_c - \mu)}) \zeta(\alpha). \quad (2.10)$$

This is a very suitable starting point for the analysis of certain properties of the partition function q . Closing the contour to the right corresponds to the large- β expansion; closing it to the left to the small- β expansion. (The relevant dimensionless expansion parameter will be made clear later). To the right of the contour the integrand in Eq. (2.10) has no poles, which means that the large- β behavior contains no inverse power in β . One might show however, that the contribution from the contour itself is not vanishing at infinity leading to exponentially damped contributions for $\beta \rightarrow \infty$, the well-known behavior of partition sums at low temperature.

However, the relevant range for the analysis of BEC is the small- β range. (As we will see we are going to obtain a reliable expansion if the de Broglie wavelength is small compared with the typical extensions of the cavity. For μm -sized cavities this will be true near the transition temperature.) Thus we close the contour to the left and pick up only the leading two terms at $\alpha = d/2$ and (for $d > 1$) $\alpha = (d-1)/2$. We find

$$\begin{aligned}
q &= q_0 + \Gamma(d/2) \beta^{-d/2} \text{Li}_{(d+2)/2}(e^{-\beta(\mu_c - \mu)}) \text{Res } \zeta(d/2) \\
&+ \Gamma\left(\frac{d-1}{2}\right) \beta^{-(d-1)/2} \text{Li}_{(d+1)/2}(e^{-\beta(\mu_c - \mu)}) \\
&\times \text{Res } \zeta((d-1)/2) + \dots, \tag{2.11}
\end{aligned}$$

with the residues of $\zeta(s)$ denoted by $\text{Res } \zeta$. The case $d=1$ is special in that $\zeta(s)$ has no pole at $s=(d-1)/2=0$. For that dimension the subleading contribution contains $\zeta'(0)$ of which, as a rule, no detailed information is available. So later, for $d=1$, we will consider only the leading contribution coming from $\text{Res } \zeta(1/2)$ and which is correctly given above.

In order to obtain a reliable approximation (in any dimension) at the critical temperature where BEC occurs we are thus left with the task of determining the leading poles of the ζ function associated with the Schrödinger equation. Concerning this determination there are deep connections between the ζ function of an operator and its heat-kernel defined as [27]

$$K(t) = \sum_N' e^{-t(E_N - \mu_c)}. \tag{2.12}$$

The small- t behavior of Eq. (2.12) is of special relevance here,

$$K(t) \sim \frac{1}{(4\pi t)^{d/2}} \sum_{l=0,1/2,1,\dots}^{\infty} a_l t^l, \tag{2.13}$$

where for a generally curved spacetime in the meantime the first 6 coefficients are known for an arbitrarily shaped smooth cavity [28] and for an arbitrary second-order elliptic operator with leading symbol the metric of the spacetime. We will need here only the first two coefficients which for the Schrödinger operator at hand read

$$a_0 = \left(\frac{2m}{\hbar^2}\right)^{d/2} V, \tag{2.14}$$

$$a_{1/2} = \left(\frac{2m}{\hbar^2}\right)^{(d-1)/2} \frac{\sqrt{\pi}}{2} (\partial V) b, \tag{2.15}$$

with V the volume of the cavity, ∂V the area of its boundary, and b being a parameter depending on the boundary conditions,

$$b = \begin{cases} -1 & \text{for Dirichlet boundary conditions} \\ 1 & \text{for Neumann boundary conditions.} \end{cases} \tag{2.16}$$

Although to the authors knowledge Neumann boundary conditions do not occur in physical applications of nonrelativistic theories considered here, we include them for mathematical completeness and because they do not lead to any extra difficulty in calculation. The relevance of Neumann boundary conditions in physics stems from the treatment of the electromagnetic field in the presence of ideal conducting plates, or the bag model in quantum chromodynamics (QCD).

As is easily seen, the residues of $\zeta(s)$, Eq. (2.8) might be expressed through the heat-kernel coefficients in Eq. (2.13). Using the integral representation for the Γ function we write

$$\zeta(s) = \frac{1}{\Gamma(s)} \sum_N' \int_0^\infty dt t^{s-1} e^{-(E_N - \mu_c)}. \tag{2.17}$$

Then we split the integral into $t \in [0,1]$ and $t \in [1,\infty)$. For the first interval we use the asymptotic expansion (2.13), the contribution from the second interval is analytic in s since the pole terms come from the $t \rightarrow 0$ behavior of the integrand. Thus we find

$$\begin{aligned}
\zeta(s) &= \frac{1}{(4\pi)^{d/2}} \frac{1}{\Gamma(s)} \sum_{l=0,1/2,1,\dots}^{\infty} a_l \int_0^1 dt t^{s-1-d/2+l} \\
&+ (\text{finite pieces}) \\
&= \frac{1}{(4\pi)^{d/2}} \frac{1}{\Gamma(s)} \sum_{l=0,1/2,1,\dots}^{\infty} \frac{a_l}{s+l-d/2} + (\text{finite pieces}) \tag{2.18}
\end{aligned}$$

and read off

$$\text{Res } \zeta(d/2) = \frac{a_0}{(4\pi)^{d/2} \Gamma(d/2)}, \tag{2.19}$$

$$\text{Res } \zeta((d-1)/2) = \frac{a_{1/2}}{(4\pi)^{d/2} \Gamma((d-1)/2)}. \tag{2.20}$$

Additional poles are located to the left of the above ones. The associated residues will depend on the details of the boundary of the cavity like its extrinsic curvature form. Having, however, current experimental situations in mind, these are probably negligible and so we are not going to present more than the subleading order in our results. In doing this, results will be very comprehensible, but let us stress that higher orders could be included easily.

Using Eqs. (2.19), (2.20), (2.14), (2.15) in the result (2.11) for the partition sum, we find to the two leading orders (as mentioned, for $d=1$, now and in the following, only the leading piece is correct and will be considered)

$$\begin{aligned}
q &= q_0 + \text{Li}_{(d+2)/2}(e^{-\beta(\mu_c - \mu)}) \frac{V}{\lambda_T^d} \\
&+ \frac{b}{4} \frac{\partial V}{\lambda_T^{d-1}} \text{Li}_{(d+1)/2}(e^{-\beta(\mu_c - \mu)}) + \dots, \tag{2.21}
\end{aligned}$$

with the de Broglie wavelength

$$\lambda_T = \frac{h}{\sqrt{2\pi m k T}}. \tag{2.22}$$

Here it is clearly seen that the expansion parameter is given by (typical extension of the cavity)/ λ_T . Our results are accurate for large values of the expansion parameter; this is, the expansion obtained is an expansion about the thermody-

nanic limit, which is the relevant one for considering BEC. It is useful to introduce the dimensionless expansion parameter

$$\xi = \frac{L}{\lambda_T} \quad (2.23)$$

with the definitions $V=L^d$ and $\partial V = \kappa L^{d-1}$. The dimensionless parameter κ contains information related to the shape of the boundary. Then Eq. (2.21) reads

$$q = q_0 + \text{Li}_{(d+2)/2}(e^{-\beta(\mu_c - \mu)}) \xi^d + \frac{\kappa b}{4} \text{Li}_{(d+1)/2}(e^{-\beta(\mu_c - \mu)}) \xi^{d-1} + \dots \quad (2.24)$$

At sufficiently low temperatures, where the ground-state population is large, the approximation $\mu \simeq \mu_c = E_0$ holds. Then using $\text{Li}_n(1) = \zeta_R(n)$, $n > 1$, Eq. (2.21) simplifies to

$$q = q_0 + \zeta_R((d+2)/2) \frac{V}{\lambda_T^d} + \frac{b}{4} \zeta_R((d+1)/2) \frac{\partial V}{\lambda_T^{d-1}} + \dots, \quad (2.25)$$

which is a very good approximation at some range below the critical temperature.

Let us now continue with the particle number,

$$N = \beta^{-1} \left(\frac{\partial q}{\partial \mu} \right) \Big|_{T,V}. \quad (2.26)$$

Here one has

$$N = N_0 + \sum'_N \frac{e^{-\beta(E_N - \mu_c)}}{1 - e^{-\beta(E_N - \mu_c)}}, \quad (2.27)$$

with the ground-state occupation number

$$N_0 = \frac{d_0}{e^{\beta(\mu_c - \mu)} - 1}. \quad (2.28)$$

(Recall that $\mu_c = E_0$.) The high-temperature expansion of N is easily obtained by noting

$$\frac{\partial \text{Li}_n(x)}{\partial x} = \frac{1}{x} \text{Li}_{n-1}(x). \quad (2.29)$$

It reads

$$N = N_0 + \text{Li}_{d/2}(e^{-\beta(\mu_c - \mu)}) \xi^d + \frac{\kappa b}{4} \text{Li}_{(d-1)/2}(e^{-\beta(\mu_c - \mu)}) \xi^{d-1} + \dots \quad (2.30)$$

The critical temperature T_c (in the absence of a phase transition) can be defined as the temperature at which the number of particles in the ground state begins to become large. We will set $N = fN_0$ with f representing the fraction of particles in the ground state. If we assume $N_0 \gg 1$, then for temperatures close to T_c we expect $\mu \simeq \mu_c$ [see Eq. (2.28)]. The behavior of the polylogarithms in Eq. (2.30) depends on the

dimension d . For $d > 3$ all of the terms in Eq. (2.30) are finite as $\mu \rightarrow \mu_c$, and we can approximate Eq. (2.30) by

$$N \simeq \zeta_R(d/2) \xi_c^d + \frac{\kappa b}{4} \zeta_R((d-1)/2) \xi_c^{d-1} + \dots \quad (2.31)$$

The critical temperature is defined via ξ_c obtained by taking $T = T_c$ in Eq. (2.23). This assumes $f \ll 1$. Defining

$$\xi_0^d = \frac{N}{\zeta_R(d/2)}, \quad (2.32)$$

which gives the critical temperature in the bulk (or thermodynamic) limit,

$$T_0 = \frac{h^2}{2\pi m k} \left(\frac{N}{V \zeta_R(d/2)} \right)^{2/d}, \quad (2.33)$$

and assuming that $\xi_c = \xi_0(1 + \gamma)$, with $\gamma \ll 1$, to leading order we can approximate (we use the temperature here)

$$T_c = T_0 \left(1 - \frac{\kappa b}{2d} \frac{\zeta_R((d-1)/2)}{\zeta_R^{(d-1)/d}(d/2)} \frac{1}{N^{1/d}} + \dots \right). \quad (2.34)$$

It is seen, that, depending on the boundary conditions imposed, the critical temperature can increase or decrease. The magnitude of the correction behaves like $N^{-1/d}$ and is typically not negligible. It is seen explicitly that the corrections are going to vanish for $N \rightarrow \infty$.

Let us now consider the lower-dimensional cases and we start with $d=3$. Then we need

$$\text{Li}_1(e^{-\beta(\mu_c - \mu)}) = -\ln[1 - (e^{-\beta(\mu_c - \mu)})]. \quad (2.35)$$

Near $\mu \simeq \mu_c$ we use Eq. (2.28) to approximate

$$\beta(\mu_c - \mu) = \ln \left(1 + \frac{1}{N_0} \right) \simeq \frac{1}{N_0}. \quad (2.36)$$

Then in three dimensions the analogue of Eq. (2.31) reads

$$N(1-f) \simeq \zeta_R(3/2) \xi^3 + \frac{\kappa b}{4} \ln(fN) \xi^2 + \dots \quad (2.37)$$

Here it is not possible to set $f=0$ in order to define a critical temperature, since in order to obtain Eq. (2.37) we have assumed $N_0 \gg 1$ [see Eq. (2.36)]. This roughly reflects the fact that in three dimensions (as well as in 1 and 2 as seen below) the number of excited states is lower than in higher dimensions, and as a result, in the temperature range considered, particles have to reside in the ground state in order that the thermodynamic equation for N is fulfilled. However, given $f \neq 0$ and N , this might be solved for the temperature,

$$T = T_0 \left\{ 1 - \frac{2}{3}(f + \alpha) \right\} \quad (2.38)$$

with

$$T_0 = \frac{h^2}{2\pi m k} \left(\frac{N}{\zeta_R(3/2)V} \right)^{2/3} \quad (2.39)$$

and

$$\alpha = \frac{\kappa b \ln(fN)}{4 \xi_R^{2/3} (3/2) N^{1/3}}, \quad (2.40)$$

valid near $\mu \simeq \mu_c$. This parallels completely Eq. (2.34). Defining the critical temperature T_c as the temperature where a given fraction f of the number of particles N is in the ground state, Eq. (2.38) can easily be used to determine T_c . This equation also shows that in the thermodynamic limit, f may be set to zero and T_0 is a ‘‘real’’ critical temperature. This reflects the fact that in three-dimensional unbounded space the ideal Bose gas exhibits Bose-Einstein condensation in the sense of a phase transition.

We proceed with $d=2$ and need in addition

$$\text{Li}_{1/2}(e^{-\beta(\mu_c - \mu)}) \simeq \sqrt{\frac{\pi}{\beta(\mu_c - \mu)}} + \dots, \quad (2.41)$$

valid for $\mu \simeq \mu_c$. Using the same approximation as before, $\beta(\mu_c - \mu) \simeq 1/N_0$, this results in

$$N(1-f) = \xi^2 \ln(fN) + \frac{\kappa b \sqrt{\pi}}{4} \xi \sqrt{fN} + \dots \quad (2.42)$$

Solving to leading order for ξ given $f \simeq 0$ we find

$$\xi_c = \sqrt{\frac{N}{\ln(fN)}} \quad (2.43)$$

or in the temperature

$$T_c = \frac{h^2}{2\pi k m} \frac{N}{\ln(fN) V}. \quad (2.44)$$

Finally in $d=1$ considering only the leading contribution results in

$$\xi_c = \sqrt{\frac{N}{\pi f}} \quad (2.45)$$

with

$$T_c = \frac{h^2}{2\pi k m} \frac{N}{\pi f V}. \quad (2.46)$$

In dimensions $d=1$ and $d=2$ it is clearly seen that we cannot set $f=0$. This reflects the fact that even in the thermodynamic limit Bose-Einstein condensation (as a phase transition) is not possible.

Another interesting quantity of the system is its internal energy defined by

$$U = \left\{ -\frac{\partial}{\partial \beta} + \frac{\mu}{\beta} \frac{\partial}{\partial \mu} \right\} q. \quad (2.47)$$

Of course the energy of the system is the sum of the single-particle energies E_N multiplied by the occupation number,

$$U = U_0 + \sum'_N E_N \frac{e^{-\beta(E_N - \mu_c)}}{1 - e^{-\beta(E_N - \mu_c)}}. \quad (2.48)$$

Here U_0 is the zero-point energy,

$$U_0 = \frac{d_0 E_0}{e^{\beta(E_0 - \mu)} - 1}. \quad (2.49)$$

To the approximation considered, U is most easily found by using Eqs. (2.11) and (2.29). As an immediate result we have

$$\begin{aligned} U &= -\frac{\partial q}{\partial \beta} + \mu N \\ &= U_0 + \frac{d}{2} \beta^{-1} \text{Li}_{(d+2)/2}(e^{-\beta(\mu_c - \mu)}) \xi^d \\ &\quad + \frac{\kappa b}{8} (d-1) \beta^{-1} \text{Li}_{(d+1)/2}(e^{-\beta(\mu_c - \mu)}) \xi^{d-1} \\ &\quad + E_0 \text{Li}_{d/2}(e^{-\beta(\mu_c - \mu)}) \xi^d \\ &\quad + E_0 \frac{\kappa b}{4} \text{Li}_{(d-1)/2}(e^{-\beta(\mu_c - \mu)}) \xi^{d-1} + \dots \end{aligned} \quad (2.50)$$

With the already presented expansions around $\mu \simeq \mu_c$ the behavior near the phase transition is easily displayed.

Finally we are left with considering the specific heat,

$$C = \left(\frac{\partial U}{\partial T} \right)_{N,V}. \quad (2.51)$$

The slightly more difficult point here is, that N has to be considered as fixed and so μ has to be considered as a function of N and β . We will need $(\partial/\partial \beta)(\beta \mu)$, which is found by differentiating Eq. (2.27) given that N is fixed,

$$\left. \frac{\partial N}{\partial \beta} \right|_{N,V} = 0. \quad (2.52)$$

Using Eq. (2.30) to the leading order, condition (2.52) yields

$$\begin{aligned} &\frac{\partial}{\partial \beta} [\beta(E_0 - \mu)] \\ &= -\frac{(d/2) \beta^{-1} \text{Li}_{d/2}(e^{-\beta(\mu_c - \mu)}) \xi^d}{(e^{-\beta(\mu_c - \mu)}) + \text{Li}_{d/2-1}(e^{-\beta(\mu_c - \mu)}) \xi^d} \\ &\quad \frac{d_0}{[1 - (e^{-\beta(\mu_c - \mu)})]^2}. \end{aligned} \quad (2.53)$$

It is seen that in the approximation $\mu = \mu_c$ one finds the above equation to yield zero as it should. Neglecting pieces coming from Eq. (2.53) (one can show that this is justified for $d < 7$) we only have to use Eq. (2.50) to find

$$\begin{aligned} \frac{C}{k} &= \frac{d}{2} \left(1 + \frac{d}{2} \right) \text{Li}_{(d+2)/2}(e^{-\beta(\mu_c - \mu)}) \xi^d \\ &\quad + \frac{\kappa b}{8} \left(\frac{d^2 - 1}{2} \right) \text{Li}_{(d+1)/2}(e^{-\beta(\mu_c - \mu)}) \xi^{d-1} + \dots, \end{aligned} \quad (2.54)$$

showing once more the decrease or increase in the specific heat depending on the boundary conditions. Using previous formulas, expansions for $\mu \approx \mu_c$ and for specific dimensions are easily found.

A slightly different treatment, which we do not pursue in this paper, could also be used. This uses the effective fugacity (for the anisotropic harmonic oscillator see [14])

$$z_{eff} = z e^{-\beta E_1}, \quad (2.55)$$

where E_1 is the first excited level with degeneracy d_1 . Whereas in the calculations presented above only the ground state has been treated separately. We can now separate the ground state and the first excited level to find

$$q = q_0 + d_1 \text{Li}_1(z_{eff}) + \text{Li}_{(d+2)/2}(z_{eff}) \frac{V}{\lambda_T^d} + \frac{b}{4} \frac{\partial V}{\lambda_T^{d-1}} \text{Li}_{(d+1)/2}(z_{eff}) + \dots$$

This expansion is a very good approximation even below the critical temperature (for the harmonic oscillator see [14]). All thermodynamical properties are obtained in the same manner as before.

III. DENSITY OF STATES METHOD

An alternative approach to the use of the Mellin-Barnes contour integral representation is to try to convert the sums for the thermodynamic quantities directly into ordinary integrals with an appropriate density of states factor. This has been widely used in a variety of problems in statistical mechanics. (See Ref. [29], for example). Recently Grossmann and Holthaus [10,11] have used such a density of states method to study the statistical mechanics of particles in a harmonic oscillator potential trap, and in a three-dimensional cubic box [16] with Dirichlet boundary conditions. The harmonic oscillator trap is characterized by a density of states

$$\rho(E) = \frac{E^2}{2\Omega^3} + \gamma \frac{E}{\Omega^2}, \quad (3.1)$$

where $\Omega = (\omega_1 \omega_2 \omega_3)^{1/3}$ is the geometric mean of the anisotropic harmonic oscillator frequencies. In Ref. [30] we showed how it is possible to evaluate γ analytically, and obtain additional corrections to Eq. (3.1) (see also [14]). The purpose of the present section is to discuss the method in greater detail in a more general setting, and to show how results equivalent to those of the previous section may be obtained with the density of states method. The basic idea behind the method can be found in Ref. [31] with a number of examples illustrated.

Suppose that we have a self-adjoint differential operator Δ that possesses a set of eigenvalues $\{\lambda_N\}$ that are all positive. Here N represents a multi-index which labels the eigenvalues. For the case of statistical mechanics in a cavity, Δ can be taken to be the Hamiltonian with λ_N the energy levels E_N . The eigenvalues depend on the details of the cavity and boundary conditions imposed, but the method we describe can be used regardless of such details. Let $\mathcal{N}(\lambda)$ be the num-

ber of modes for the boundary value problem in the cavity for which the eigenvalues $\lambda_N \leq \lambda$. We can write

$$\mathcal{N}(\lambda) = \sum_N \theta(\lambda - \lambda_N), \quad (3.2)$$

where $\theta(x)$ is the Heaviside distribution (or step function) defined by

$$\theta(x) = \begin{cases} 1, & x > 0, \\ 0, & x < 0, \\ \frac{1}{2}, & x = 0. \end{cases} \quad (3.3)$$

This gives the result

$$\mathcal{N}(\lambda) = \sum_{\lambda_N < \lambda} 1 + \sum_{\lambda_N = \lambda} \frac{1}{2}, \quad (3.4)$$

as used by Baltes and Hilf [31].

The aim now is to treat the eigenvalues as a continuous distribution rather than a discrete set by introducing the eigenvalue (or spectral) density $\rho(\lambda)$. We define

$$\rho(\lambda) d\lambda = \mathcal{N}(\lambda + d\lambda) - \mathcal{N}(\lambda) \quad (3.5)$$

$$\simeq \frac{d\mathcal{N}(\lambda)}{d\lambda} d\lambda. \quad (3.6)$$

Use of Eq. (3.2) for $\mathcal{N}(\lambda)$, along with the distributional identity $\theta'(x) = \delta(x)$ gives

$$\rho(\lambda) = \sum_N \delta(\lambda - \lambda_N). \quad (3.7)$$

If we use the familiar exponential representation for the Dirac δ distribution, then

$$\rho(\lambda) = \sum_N \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ik(\lambda - \lambda_N)} = \sum_N \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} dt e^{t(\lambda - \lambda_N)}. \quad (3.8)$$

We may now translate the integration contour in Eq. (3.8) to the right by an amount c where $c \in \mathbb{R}$ with $c > 0$, and assume that we are permitted to interchange the order of the summation and integration. This results in

$$\rho(\lambda) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} dt e^{t\lambda} K(t), \quad (3.9)$$

where

$$K(t) = \sum_N e^{-t\lambda_N}. \quad (3.10)$$

Equation (3.9) shows that $\rho(\lambda)$ is the inverse Laplace transform of $K(t)$. Inversion of Eq. (3.9) results in

$$K(t) = \int_0^{\infty} d\lambda e^{-t\lambda} \rho(\lambda). \quad (3.11)$$

Another way of arriving at Eq. (3.9) is to note that Eq. (3.11) follows directly from Eqs. (3.7) and (3.10), establishing that $\rho(\lambda)$ is the Laplace transform of $K(t)$. The inversion formula for Laplace transforms gives Eq. (3.9) immediately without the intermediate steps in Eq. (3.8).

The point of Eqs. (3.9) and (3.11) is that given $K(t)$ as defined in Eq. (3.10) we can evaluate the density of states in a straightforward way. In certain simple cases, such as the harmonic oscillator potential, where the eigenvalues can be written down explicitly, it is possible to perform the sum in Eq. (3.10) and evaluate $K(t)$ in closed form (see Ref. [30] for a case of this). In the generic case, where the eigenvalues are not known explicitly, we can still obtain a result for the density of states by using the known asymptotic expansion for $K(t)$ as $t \rightarrow 0$ [27].

Assume that as $t \rightarrow 0$ we have the generic expansion

$$K(t) \approx \sum_{i=1}^k c_i t^{-r_i} + \mathcal{O}(t^{-r_{k+1}}) \quad (3.12)$$

for some coefficients c_i and powers r_i with $r_1 > r_2 > \dots > r_k$. The simplest way to evaluate $\rho(\lambda)$ is to use Eq. (3.11) and the relation

$$t^{-z} = \frac{1}{\Gamma(z)} \int_0^\infty d\lambda \lambda^{z-1} e^{-t\lambda}, \quad (3.13)$$

which is valid for $\text{Re } z > 0$. It is now easy to see that

$$\rho(\lambda) \approx \sum_{i=1}^k \frac{c_i}{\Gamma(r_i)} \lambda^{r_i-1}. \quad (3.14)$$

Integrating this result with respect to λ results in

$$\mathcal{N}(\lambda) \approx \sum_{i=1}^k \frac{c_i}{\Gamma(r_i+1)} \lambda^{r_i}. \quad (3.15)$$

Although the analysis that have presented makes no attempt at proper mathematical rigour, the main result in Eq. (3.14) of (3.15) is in agreement with a refinement of Karamata's theorem due to Brownell [32] (a nice account is contained in Ref. [31]). It is important to emphasize that the result for $\rho(\lambda)$ or $\mathcal{N}(\lambda)$ refers really to the average number of eigenvalues. Generally the number will fluctuate around some average value. These fluctuations can be important in some contexts [31,33]. Another point worth stressing is that our results have assumed that r_k in Eq. (3.12) is positive. The results (3.14) and (3.15) are actually true for all r_k if we define $1/\Gamma(r_i) = 0$ when $r_i = 0, -1, -2, \dots$. The establishment of this result requires a more powerful approach than Laplace transforms [32].

The density of states (3.14) is determined by a knowledge of the coefficients c_i appearing in the asymptotic expansion of $K(t)$. These coefficients can be evaluated from a knowledge of the generalized ζ function associated with the eigenvalues λ_N as discussed in the previous section. Defining

$$\zeta(s) = \sum_N \lambda_N^{-s}, \quad (3.16)$$

the analysis in Sec. II is easily modified to show that $\zeta(s)$ has a simple pole at $s = r_i$ with residue

$$\text{Res } \zeta(s)|_{s=r_i} = \frac{c_i}{\Gamma(r_i)} \quad (3.17)$$

for $r_i \neq 0, -1, -2, \dots$; and

$$\zeta(s = -r_i) = (-1)^{r_i} (-r_i)! c_i \quad (3.18)$$

for $r_i = 0, -1, -2, \dots$. Therefore the coefficients c_i appearing in the density of states may also be found from a knowledge of the generalized ζ function. This provides a direct link between the density of states approach and the method described in Sec. II.

We will conclude this section by showing how the density of states method may be used in the specific case of an ideal gas confined in a general cavity. The q potential defined earlier was written as

$$q = q_0 + q_{ex}, \quad (3.19)$$

where

$$q_0 = -d_0 \ln(1 - z e^{-\beta E_0}) \quad (3.20)$$

was the ground-state contribution, and

$$q_{ex} = \sum_{n=1}^{\infty} \frac{e^{n\beta(\mu - \mu_c)}}{n} \sum_N' e^{-n\beta(E_N - E_0)} \quad (3.21)$$

represents the contribution from the excited states. The sum over energy levels in Eq. (3.21) can now be converted into an integral over a continuous energy variable by introducing a density of states factor. From Eq. (3.14) and using the coefficients c_i found in Sec. II we have

$$\rho(E) \approx \frac{V \beta^{d/2} E^{d/2-1}}{\lambda_T^d \Gamma(d/2)} + \frac{b}{4} \frac{(\partial V) \beta^{(d-1)/2} E^{(d-3)/2}}{\lambda_T^{d-1} \Gamma((d-1)/2)} \quad (3.22)$$

if we keep only the first-order correction to the bulk expression as before. To this order we may approximate

$$q_{ex} \approx \sum_{n=1}^{\infty} \frac{e^{n\beta(\mu - \mu_c)}}{n} \int_{E_1 - E_0}^{\infty} dE \rho(E) e^{-n\beta E}. \quad (3.23)$$

Replacing the lower limit in the integration with 0, we obtain

$$q_{ex} \approx \lambda_T^{-d} V \text{Li}_{(d+2)/2}(e^{-\beta(\mu_c - \mu)}) + \frac{b}{4} \lambda_T^{-(d-1)} (\partial V) \text{Li}_{(d+1)/2}(e^{-\beta(\mu_c - \mu)}) \quad (3.24)$$

in agreement with our earlier method. The replacement of the lower limit on the integral with 0 assumes $\beta E_0 \ll 1$ so that the temperature is well above the temperature associated with the ground-state energy (i.e., $kT \gg E_0$.) If the energy gap $E_1 - E_0$ is of the same order of magnitude as the ground-state energy, then $\beta E_1 \ll 1$ as well. Results for the particle number and other thermodynamic quantities follow as before.

IV. APPLICATION OF THE RESULTS TO SOME CAVITIES

This section will discuss some specific examples like the rectangular box and the spherical cavity with various boundary conditions. The rectangular box has been the subject of considerable investigation. (See Refs. [34,35] for reviews.) In order to get all thermodynamic quantities as derived in Secs. II and III, we only need to give the constant b , the volume of the cavity V , and the boundary ∂V . Another interesting quantity is the lowest-energy eigenvalue as the critical value for the chemical potential.

A. Rectangular box

For the rectangular box with side lengths L_1, \dots, L_d one can consider, for example, periodic, Dirichlet, and Neumann boundary conditions. In Cartesian coordinates $x = (x_1, \dots, x_d)$ with $x_i \in [0, L_i]$.

For periodic boundary conditions,

$$\phi(x_1, \dots, x_i, \dots, x_d) = \phi(x_1, \dots, x_i + L_i, \dots, x_d), \quad (4.1)$$

with $i = 1, \dots, d$, the energy eigenvalues are

$$E_{n_1, \dots, n_d} = \sum_{i=1}^d \left(\frac{2\pi}{L_i} n_i \right)^2, \quad n_i \in \mathbb{Z}. \quad (4.2)$$

Periodic identification means that effectively there is no boundary. (Equivalently we can regard V as the d torus.) In this case $b = 0$. Furthermore, one has for the volume

$$V_d = \prod_{i=1}^d L_i \quad (4.3)$$

and $\mu_c = E_0 = 0$.

For Dirichlet boundary conditions,

$$\phi(x_1, \dots, x_{i-1}, 0, x_{i+1}, \dots, x_d) = 0,$$

$$\phi(x_1, \dots, x_{i-1}, L_i, x_{i+1}, \dots, x_d) = 0,$$

one gets

$$E_{n_1, \dots, n_d} = \sum_{i=1}^d \left(\frac{\pi n_i}{L_i} \right)^2, \quad n_i \in \mathbb{N}. \quad (4.4)$$

As mentioned, see Eq. (2.16), $b = -1$, the volume is as before and, furthermore,

$$\partial V = 2 \sum_{i=1}^d V_{d-1}^{(i)}. \quad (4.5)$$

Here, $V_{d-1}^{(i)}$ is the volume of the i th side of the rectangular cavity, $V_{d-1}^{(i)} = L_1 \cdots L_{i-1} L_{i+1} \cdots L_d$. Furthermore,

$$E_0 = \sum_{i=1}^d \left(\frac{\pi}{L_i} \right)^2. \quad (4.6)$$

If we specialize to the d cube, then $\partial V = 2dL^{d-1}$ which gives $\kappa = 2d$.

Finally, for Neumann boundary conditions,

$$(\partial/\partial x_i) \phi(x_1, \dots, x_d)|_{x_i=0} = 0,$$

$$(\partial/\partial x_i) \phi(x_1, \dots, x_d)|_{x_i=L_i} = 0,$$

the energy eigenvalues read

$$E_{n_1, \dots, n_d} = \sum_{i=1}^d \left(\frac{\pi n_i}{L_i} \right)^2, \quad n_i \in \mathbb{N}_0, \quad (4.7)$$

with $\mu_c = E_0 = 0$, $b = 1$ and V , ∂V , as before.

All thermodynamical quantities may now be given immediately with the formulas in Sec. II. Especially for the critical temperature one has that periodic boundary conditions give a critical temperature identical to the thermodynamic limit (a result of being no boundary there), Dirichlet boundary conditions increase it and Neumann boundary conditions decrease it.

Looking at the distribution of the eigenvalues around the ground state of the system an intuitive explanation of this behavior is possible. Let us assume for this equal compactification sides L_i . It is clear that the lower the density of eigenvalues near the ground state the higher the transition temperature will be. Then the following might be stated. Neumann boundary conditions lead to the lowest condensation temperature because it has the smallest spacing between the ground state and the first excited level. This compensates the doubled number of eigenstates in the periodic case, the eigenvalues that are, however, four times higher. The difference between Neumann and Dirichlet boundary conditions is based on the same observation; in addition the degeneracy of the eigenvalues is the same for these two boundary conditions. The difference between periodic and Dirichlet boundary conditions is not obvious; however, the results show that the slightly smaller level spacing for Dirichlet boundary conditions is more than compensated by the doubling of the degeneracy for periodic boundary conditions.

B. Spherical cavities

For spherical cavities an explicit knowledge of the eigenvalues is not at hand and for that reason also a numerical treatment of the partition sum is not immediate. For this kind of example our analytical approach is most useful.

It is convenient to introduce a spherical coordinate basis, with $r = |x|$ and $d-1$ angles $\Omega = (\theta_1, \dots, \theta_{d-2}, \varphi)$. In these coordinates, a complete set of solutions of the Schrödinger equation together with one of the mentioned boundary conditions may be given in the form

$$\phi_{l,m,n}(r, \Omega) = r^{1-(d/2)} J_{l+[(d-2)/2]}(\sqrt{2m} w_{l,n} r / \hbar) Y_{l+[(d/2)]}(\Omega), \quad (4.8)$$

with $J_{l+[(d-2)/2]}$ being Bessel functions and $Y_{l+[(d/2)]}$ hyperspherical harmonics [36]. Here, $E_{l,n} = w_{l,n}^2$ and the $w_{l,n} (> 0)$ are determined through the boundary conditions by

$$J_{l+[(d-2)/2]}(\sqrt{2m} w_{l,n} R / \hbar) = 0 \quad (4.9)$$

for Dirichlet boundary conditions and

$$0 = \frac{1-d/2}{R} J_{l+[(d-2)/2]}(\sqrt{2mw_{l,n}}R/\hbar) + \frac{\sqrt{2mw_{l,n}}}{\hbar} J'_{l+[(d-2)/2]}(\sqrt{2mw_{l,n}}r/\hbar)|_{r=R}$$

for Neumann boundary conditions. Although none of these eigenvalues is known explicitly, in order to obtain an approximation of all thermodynamic quantities, it is already enough to state the volume and the boundary volume of the spherical cavity,

$$V = \frac{\pi^{d/2} R^d}{\Gamma(d/2+1)}, \quad \partial V = \frac{2\pi^{d/2} R^{d-1}}{\Gamma(d/2)}, \quad (4.10)$$

and to apply the results of the previous sections.

V. DISCUSSION AND CONCLUSIONS

We have described two methods for treating the ideal Bose gas using the grand canonical ensemble in a general cavity. The first method, described in Sec. II, treats the partition function as a sum over the discrete energy levels by making use of the Mellin-Barnes integral representation for the exponential function. The second method shows how to obtain an adequate density of states factor so that the sum

over discrete energy levels can be replaced with an integral. Both methods make use of the so-called heat-kernel coefficients for the Schrödinger operator, and equivalence between the two methods is shown in quite a general setting.

Our analysis shows clearly the way in which the geometry of the cavity enters in all thermodynamic properties. In the limit considered, namely, $\xi = L/\lambda_T \gg 1$, the leading correction to the bulk limit term ξ^d enters via the property $\kappa = (\partial V)/V^{(d-1)/d}$. Thus the leading-order correction is completely described by the volume and area of the cavity, with all finer details washed out for $\xi \gg 1$. Finer detail would be present in the next to subleading order in terms of the extrinsic curvature of the boundary. (The extrinsic curvature describes how the normal vector to the boundary varies when moving along the boundary.)

These ideas are as well applicable to the canonical ensemble. Furthermore, due to the connections between the microcanonical and the grand canonical approach stated recently in [37–39] it seems possible to develop this approach also for the microcanonical ensemble.

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