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Master equation vs. partition function: canonical statistics of ideal Bose–Einstein condensates

Martin Holthaus[a,*], Kishore T. Kapale[b,c], Vitaly V. Kocharovsky[b,d], Marlan O. Scully[b,c]

[a] *Fachbereich Physik, Carl von Ossietzky Universität, D-26111 Oldenburg, Germany*

[b] *Department of Physics and Institute for Quantum Studies, Texas A&M University, College Station, TX 77843, USA*

[c] *Max-Planck-Institut für Quantenoptik, D-85748 Garching, Germany*

[d] *Institute of Applied Physics of the Russian Academy of Science, 603600 Nizhny Novgorod, Russia*

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Abstract

Within the canonical ensemble, a partially condensed ideal Bose gas with arbitrary single-particle energies is equivalent to a system of uncoupled harmonic oscillators. We exploit this equivalence for deriving a formula which expresses all cumulants of the canonical distribution governing the number of condensate particles in terms of the poles of a generalized Zeta function provided by the single-particle spectrum. This formula lends itself to systematic asymptotic expansions which capture the non-Gaussian character of the condensate fluctuations with utmost precision even for relatively small, finite systems, as confirmed by comparison with exact numerical calculations. We use these results for assessing the accuracy of a recently developed master equation approach to the canonical condensate statistics; this approach turns out to be quite accurate even when the master equation is solved within a simple quasithermal approximation. As a further application of the cumulant formula we show that, and explain why, all cumulants of a homogeneous Bose–Einstein condensate "in a box" higher than the first retain a dependence on the boundary conditions in the thermodynamic limit. © 2001 Elsevier Science B.V. All rights reserved.

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* Corresponding author. Tel.: +49-441-798-3960.
E-mail address: holthaus@marvin.physik.uni-oldenburg.de (M. Holthaus).

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1. Introduction

It sometimes happens that a problem in physics can be solved by two quite different methods, each one requiring its own propositions and approximations. In such a case it can be rewarding to compare these two approaches in some detail: What is hard to derive within the first approach might be obvious within the second; both methods might lend themselves to different generalizations. In such a comparison it is not so much the result itself that matters, but rather the "best" way to obtain it; the hope is that a thorough understanding of the solution techniques will provide a key for attacking more demanding problems.

Such a situation arises when studying the ideal Bose gas in the canonical ensemble. While the *grand* canonical treatment of ideal Bose gases constitutes classic textbook material [1–3], recent experiments with mesoscopic samples of dilute Bosonic atoms in thermally isolated traps (for a Review, see Ref. [4]) actually call for a microcanonical analysis. The canonical ensemble provides a convenient intermediate step: It still assumes that the trapped gas exchanges energy with a heat bath, as in a grand canonical setting, but it embodies the constraint that the number of gas particles, N, be fixed. Experiments with ^{4}He in a porous medium [5] provide an interesting example of Bose–Einstein condensation in the canonical ensemble.

One approach to the canonical statistics of ideal Bose gases, presented in Ref. [6] and developed further in Ref. [7], consists in setting up a master equation for the condensate and finding its equilibrium solution. This approach has the merit of being technically lucid and physically illuminating, since it reveals important parallels to the quantum theory of the laser [8]. For deriving that master equation, in the approximation of detailed balance in the excited states, it was assumed that given an arbitrary number n_0 of atoms in the condensate, the remaining $N - n_0$ excited atoms are in an equilibrium state at the prescribed temperature T—or, in other words, that the occupation numbers of the excited-states subsystem thermalize significantly faster than the condensed ones, no matter how many particles the condensate contains. Whereas the existence of two separate time scales is evident in laser physics, where the atomic dynamics usually are fast compared to the escape of photons from the cavity, the physical motivation for such a separation of time scales seems less obvious in the present case. However, it was shown [9] that indeed the time scale of long-range coherent ordering is much greater than the collisional time scale responsible for the kinetic equilibration of above-condensate atoms. Thus, while this assumption might not be sufficient for describing the details of the process of equilibration, it does lead, in principle, to the correct canonical-ensemble equilibrium state [10]. Still, for evaluating that equilibrium state one has to make certain additional approximations, as detailed in Section 2, so that it is desirable to check conclusions drawn from the master equation approach against the results provided by independent techniques.

A classic technique that almost seems to suggest itself for studying canonical statistics is the saddle-point method: Starting from the known grand canonical partition function one employs the saddle-point approximation for extracting its required canonical counterpart, which then yields all desired quantities by taking suitable derivatives. It turns out that this program requires some caution, since the customary form of the saddle-point approximation, as advocated by Schrödinger in his famous treatise [11], is not correct in the condensate regime; the close approach of the saddle-point to the ground-state singularity of the grand partition function forbids the usual Gaussian approximation. Fortunately, this difficulty can be overcome with the help of a strategy that has been suggested by Dingle [12] and worked out in detail in Refs. [13,14]; this approach furnishes canonical occupation numbers and their fluctuations, say, for reasonably large, experimentally relevant particle numbers N and *all* temperatures. However, accurately solving the equation for the saddle-point requires some numerical skills.

In this paper, therefore, we will follow still another avenue for checking the master equation approach. Instead of aiming for approximations valid at all temperatures—as provided by the proper saddle-point method—we will restrict ourselves to temperatures below the onset of Bose–Einstein condensation. In this case there exists a transparent approximation which allows us to bring the canonical partition function into a simple form—namely into that of a system of independent harmonic oscillators [15–18]. Using this, we derive a formula which expresses all the cumulants $\kappa_k(\beta)$ of the canonical distribution $p_N^{(\mathrm{ex})}(M;\beta)$—i.e., the probability distribution for finding M of the N atoms in an excited state at inverse temperature β, and hence $n_0 = N - M$ atoms in the condensate—in terms of the poles of a generalized Zeta function determined by the system's single-particle energies. This result is of substantial interest, since systems that lend themselves to an explicit calculation of all higher moments beyond the usual Gaussian second order are quite rare in physics. Our approach enables us, first of all, to make contact with the master equation, and to disperse possible objections against it: The first and the second moment of $p_N^{(\mathrm{ex})}(M;\beta)$, as obtained from the master equation within a "quasithermal" approximation, merge *exactly* into the corresponding results provided by the bona fide partition function; the higher moments are systematically approximated in a mean field-like fashion. The Zeta-function technique also allows us to clarify an important issue: In the case of the homogeneous Bose gas "in a box", the "higher" statistical properties (i.e., the cumulants $\kappa_k(\beta)$ with order $k \geqslant 2$) do depend on the particular boundary conditions even in the thermodynamic limit. When it comes to a detailed discussion of the statistics of occupation numbers, simply taking the homogeneous Bose gas with the convenient periodic boundary conditions might, therefore, not be sufficient.

We restrict this paper to the discussion of orthodox equilibrium statistical mechanics and do not consider the method of canonical quasiparticles, which was introduced [17,18] on the basis of a particle-number conserving formalism established by Girardeau and Arnowitt [19,20]. That method is very efficient for the solution of various non-equilibrium problems in the canonical ensemble, such as the dynamics of condensate formation, vortex evolution, and the kinetics of correlations, both for the ideal and the interacting Bose gas.

The main part of this paper is organized as follows: In Section 2, we summarize the master equation approach [6,7], to the extent that it will be needed later. In Section 3, we then explain why the canonical partition function of the ideal Bose gas reduces in the condensate regime to a partition function of independent harmonic oscillators, and quantify the accuracy of the master equation by comparing the canonical cumulants $\kappa_k(\beta)$ obtained from this approach with those following from the "independent oscillator" point of view, and with results of exact numerical calculations. In Section 4, we elaborate the connection between the cumulants and the poles of the generalized Zeta functions, while Section 5 contains the explicit evaluation of our general formula for an isotropic harmonic trapping potential, and for the "box" potential with periodic or Dirichlet boundary conditions, respectively. The detailed analysis of the higher cumulants, in particular, of those of third and fourth order (skewness and flatness), yields interesting insight into the non-Gaussian nature of the condensate fluctuations. A brief discussion concludes the paper in Section 6. Since the required techniques for handling the generalized Zeta functions might not be generally known, and in order to keep the paper self-contained, Appendix A offers the relevant mathematical details.

2. Essentials of the master equation approach

We consider an ideal Bose gas that consists of N particles and is stored in some arbitrary trap. The trapping potential determines the discrete single-particle energies ε_ν; the index $\nu = 0, 1, 2, \ldots$ labels the individual single-particle eigenstates. It is further assumed that this system is kept in thermal contact with a harmonic-oscillator heat bath of temperature T; at sufficiently low T a fraction of the particles undergoes Bose–Einstein condensation and occupies the ground state $\nu = 0$. We require that the spectral density of the bath be flat, so that for each transition of a gas particle, involving an energy difference $\varepsilon_\nu - \varepsilon_\sigma$, there is always the same number of frequency-matched oscillators which can provide or accept this quantum. The average occupation number of such a heat-bath oscillator is written as

$$\eta_{\nu\sigma} = \frac{1}{\exp[\beta(\varepsilon_\nu - \varepsilon_\sigma)] - 1} , \tag{1}$$

where $\beta = 1/k_B T$, with k_B denoting Boltzmann's constant.

Starting from the equation of motion for the total density matrix, tracing out the bath degrees of freedom in the usual manner, and making the Markov approximation of very fast relaxation in the bath compared to the dynamics of the system of excited and condensed Bose particles in the trap, one obtains a master equation for the Bose gas. This equation can be further reduced to a master equation for the condensate alone, if one assumes that the state of the excited particles is determined by detailed balance [6,7]. The condensate master equation describes the evolution of the probability p_{n_0} that the condensate contains n_0 out of the N particles, and includes information about the excited-state occupations only through the "cooling coefficients"

$$K_{n_0} = \sum_{\nu \geqslant 1} (\eta_{\nu 0} + 1)\langle n_\nu \rangle_{n_0} \tag{2}$$

and the "heating coefficients"

$$H_{n_0} = \sum_{v \geqslant 1} \eta_{v0}(\langle n_v \rangle_{n_0} + 1)\,, \tag{3}$$

where $\langle n_v \rangle_{n_0}$ is the canonical expectation value for the number of particles occupying the vth excited state, subject to the condition that there be n_0 condensate atoms. In terms of these coefficients, the master equation reads

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\, p_{n_0} = -\kappa\{&K_{n_0}(n_0+1)p_{n_0} - K_{n_0-1}n_0\, p_{n_0-1} + H_{n_0}n_0\, p_{n_0}\\ &-H_{n_0+1}(n_0+1)p_{n_0+1}\}\,.\end{aligned} \tag{4}$$

The constant κ obviously carries the dimension of an inverse time. It embodies the spectral density of the bath and the coupling strength of the bath oscillators to the gas particles [7], and determines the rate of condensate evolution since there is no direct interaction between the particles of an ideal Bose gas. Here, as in Ref. [7], we study the equilibrium solution of Eq. (4), so that the question how fast the equilibration proceeds is not important.

The content of this master equation (4) can be grasped in an intuitive manner, even without a formal derivation. The cooling coefficient K_{n_0} describes all those processes that add another particle to a condensate consisting so far of n_0 atoms: The new particle originates from one of the excited states $v \geqslant 1$, each of them endowed with the occupation number $\langle n_v \rangle_{n_0}$. The particle's transition to the ground state is accompanied by the emission of a phonon of energy $\varepsilon_v - \varepsilon_0$ into the heat bath, as expressed by the additional factor $(\eta_{v0}+1)$ in Eq. (2). Likewise, the heating coefficient (3) summarizes all those processes through which an n_0-particle condensate loses one of its constituents: By absorbing a phonon with the appropriate energy from the heat bath (—multiplicity factor η_{v0}—), the particle can make a transition to any of the excited states. Since, prior to the arrival of the new particle, the occupation number of such a state was $\langle n_v \rangle_{n_0}$, the factor $(\langle n_v \rangle_{n_0} + 1)$ properly accounts for the "emission" of the new particle into this mode. As indicated in Fig. 1, there are four contributions that affect the rate of change of p_{n_0}: an (n_0-1)-particle condensate acquiring an additional particle through cooling, an (n_0+1)-particle condensate losing one particle through heating, and an n_0-particle condensate either picking up or losing one particle; these four contributions make up the right-hand side of Eq. (4).

The above discussion also highlights an important difference between the canonical ensemble studied here and a microcanonical ensemble. In a canonical setting, the energy of each transition from or to the condensate is provided or accepted by the heat bath, implying that such transitions do not lead to correlations among the other gas particles. This is no longer the case under microcanonical conditions; here each amount of energy associated with a particle's transition to or from the condensate has to be compensated by the other particles themselves. Assuming the presence of an external heat bath enormously simplifies the analysis, but it also affects the results: For instance, microcanonical fluctuations of the number of condensate particles are smaller than their canonical counterparts [16,21].

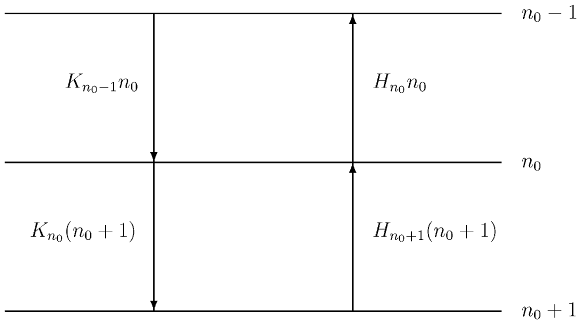

Fig. 1. Visualization of the condensate master equation (4). There are four contributions that affect the rate of change of p_{n_0}, the probability of finding n_0 particles in the condensate: An $(n_0 - 1)$-particle condensate (upper horizontal line) gaining one particle through cooling (upper downward arrow), an (n_0+1)-particle condensate (lower horizontal line) losing one particle through heating (lower upward arrow), and an n_0-particle condensate gaining or losing one constituent. These four contributions add up to give the right-hand side of Eq. (4).

For evaluating the master equation (4), one now needs an approximation to the cooling and heating coefficients (2) and (3). In Ref. [7], a quasithermal approximation for the conditional occupation numbers of the excited states was suggested:

$$\langle n_v \rangle_{n_0} = (N - n_0)\frac{\eta_{v0}}{\mathscr{H}} , \tag{5}$$

where

$$\mathscr{H} = \sum_{v \geqslant 1} \eta_{v0} = \sum_{v \geqslant 1} \frac{1}{\exp[\beta(\varepsilon_v - \varepsilon_0)] - 1} . \tag{6}$$

Summing Eq. (5) over $v \geqslant 1$, one finds

$$\sum_{v \geqslant 1} \langle n_v \rangle_{n_0} = N - n_0 , \tag{7}$$

so that this ansatz incorporates the particle number constraint in an exact manner; moreover, $\langle n_v \rangle_{n_0}$ is taken to be proportional to the phonon occupation number η_{v0}. Within this approximation, the cooling coefficient (2) is given by

$$\begin{aligned} K_{n_0} &= \sum_{v \geqslant 1} \eta_{v0} \langle n_v \rangle_{n_0} + (N - n_0) \\ &\equiv (1 + \eta)(N - n_0) , \end{aligned} \tag{8}$$

where the "cross-excitation parameter" [7]

$$\begin{aligned} \eta &= \frac{1}{N - n_0} \sum_{v \geqslant 1} \eta_{v0} \langle n_v \rangle_{n_0} = \frac{1}{\mathscr{H}} \sum_{v \geqslant 1} \eta_{v0}^2 \\ &= \frac{1}{\mathscr{H}} \sum_{v \geqslant 1} \frac{1}{(\exp[\beta(\varepsilon_v - \varepsilon_0)] - 1)^2} \end{aligned} \tag{9}$$

has been introduced. Likewise, Eq. (3) now yields

$$H_{n_0} = \mathscr{H} + (N - n_0)\eta \, . \tag{10}$$

With these approximations (8) and (10), the steady-state solution

$$p_{n_0} = \prod_{i=n_0}^{N-1} \frac{H_{i+1}}{K_i} \, p_N \tag{11}$$

to the condensate master equation (4) takes the form

$$p_{n_0} = \frac{1}{Z_N} \binom{\mathscr{H}/\eta + N - n_0 - 1}{N - n_0} \left(\frac{\eta}{1+\eta}\right)^{N-n_0} , \tag{12}$$

with $Z_N = 1/p_N$ fixed through the normalization condition $\sum_{n_0=0}^{N} p_{n_0} = 1$, giving the formal representation

$$Z_N = \sum_{n_0=0}^{N} \binom{\mathscr{H}/\eta + N - n_0 - 1}{N - n_0} \left(\frac{\eta}{1+\eta}\right)^{N-n_0} \tag{13}$$

of the canonical partition function. Interestingly, the distribution (12) closely resembles a negative binomial distribution; the only difference lies in the fact that here $N - n_0$ is restricted to integers in the range from 0 to N, whereas all non-negative integers figure in the true negative binomial case. All moments of this distribution (12) can be calculated analytically. In particular, one finds

$$\begin{aligned}\langle n_0 \rangle &= \sum_{n_0=0}^{N} n_0 \, p_{n_0} \\ &= N - \mathscr{H} + p_0(\mathscr{H} + \eta N)\end{aligned} \tag{14}$$

as the canonical expectation value of the number of condensate particles; its variance

$$\begin{aligned}\Delta n_0^2 &= \langle n_0^2 \rangle - \langle n_0 \rangle^2 \\ &= (1+\eta)\mathscr{H} - p_0(\mathscr{H} + \eta N)(1 + \eta - \mathscr{H} + N) - p_0^2(\mathscr{H} + \eta N)^2 \, ,\end{aligned} \tag{15}$$

the third centered moment

$$\begin{aligned}\langle (n - \langle n_0 \rangle)^3 \rangle = &-(1+\eta)(1+2\eta)\mathscr{H} \\ &+ p_0(\mathscr{H} + \eta N)[1 + (\mathscr{H} - N)^2 + 2(\eta^2 + N(1+\eta)) \\ &+ 3(\eta - \mathscr{H}(1+\eta))] + 3\,p_0^2(\mathscr{H} + \eta N)^2(1 + \eta - \mathscr{H} + N) \\ &+ 2\,p_0^3\,(\mathscr{H} + \eta N)^3 \, ,\end{aligned} \tag{16}$$

and the fourth centered moment

$$\begin{aligned}\langle (n - \langle n_0 \rangle)^4 \rangle = &(1+\eta)[1 + 3(1+\eta)(\mathscr{H} + 2\eta)]\mathscr{H} \\ &- p_0(\mathscr{H} + \eta N)[1 - \mathscr{H} + 3(1 + \eta - \mathscr{H} + N)(N + 2\eta^2)\end{aligned}$$

$$- (\mathscr{H} - N)^3 + \eta(7 - 3(N+2)(\mathscr{H} - N) + \eta(\mathscr{H} + 6))]$$
$$- 2p_0^2(\mathscr{H} + \eta N)^2[2 + 2(\mathscr{H} - N)^2 + 4(\eta^2 + N(1+\eta))$$
$$+ 3(2\eta - \mathscr{H}(1+\eta))] - 6p_0^3(\mathscr{H} + \eta N)^3(1 + \eta - \mathscr{H} + N)$$
$$- 3p_0^4(\mathscr{H} + \eta N)^4 . \quad (17)$$

Thus, assuming the validity of the quasithermal approximation (5), the master equation (4) provides a complete description of the canonical statistics of ideal Bose–Einstein condensates.

For later reference, let us specialize the moments (14)–(17) to the condensate regime, that is, to temperatures so low that p_0, the probability for finding no particle at all in the ground state, is practically zero. Recall first that within the *grand* canonical ensemble the occupation numbers take the form $\langle n_v \rangle^{\text{gc}} = [z^{-1}\exp(\beta\varepsilon_v) - 1]^{-1}$, with the fugacity z being tied to the ground state energy, $z \approx \exp(\beta\varepsilon_0)$. Since for large N these grand canonical occupation numbers equal their canonical counterparts $\langle n_v \rangle$ (where the absence of the index n_0 distinguishes these expectation values from the conditional occupation numbers entering the heating and cooling coefficients (2) and (3)), one has

$$\langle n_v \rangle = \frac{1}{\exp[\beta(\varepsilon_v - \varepsilon_0)] - 1} \quad \text{in the condensate regime} , \quad (18)$$

so that the parameters $\mathscr{H}$ and η, defined in Eqs. (6) and (9), can be expressed through these occupation numbers $\langle n_v \rangle$ as

$$\mathscr{H} = \sum_{v \geqslant 1} \langle n_v \rangle \quad \text{and} \quad \eta = \frac{\sum_{v \geqslant 1} \langle n_v \rangle^2}{\sum_{v \geqslant 1} \langle n_v \rangle} . \quad (19)$$

Accordingly, taking the limit $p_0 \to 0$, we obtain for the centered moments

$$\langle n_0 \rangle = N - \mathscr{H} = N - \sum_{v \geqslant 1} \langle n_v \rangle , \quad (20)$$

$$\Delta n_0^2 = (1+\eta)\mathscr{H} = \sum_{v \geqslant 1} \langle n_v \rangle(\langle n_v \rangle + 1) , \quad (21)$$

$$\begin{aligned} \langle (n_0 - \langle n_0 \rangle)^3 \rangle &= -(1+\eta)(1+2\eta)\mathscr{H} \\ &= -\sum_{v \geqslant 1} \langle n_v \rangle - 3\sum_{v \geqslant 1} \langle n_v \rangle^2 - 2\frac{(\sum_{v \geqslant 1} \langle n_v \rangle^2)^2}{\sum_{v \geqslant 1} \langle n_v \rangle} , \end{aligned} \quad (22)$$

$$\begin{aligned} \langle (n_0 - \langle n_0 \rangle)^4 \rangle &= (1+\eta)(1+6\eta+6\eta^2)\mathscr{H} + 3[(1+\eta)\mathscr{H}]^2 \\ &= \sum_{v \geqslant 1} \langle n_v \rangle + 7\sum_{v \geqslant 1} \langle n_v \rangle^2 + 12\frac{(\sum_{v \geqslant 1} \langle n_v \rangle^2)^2}{\sum_{v \geqslant 1} \langle n_v \rangle} \\ &\quad + 6\frac{(\sum_{v \geqslant 1} \langle n_v \rangle^2)^3}{(\sum_{v \geqslant 1} \langle n_v \rangle)^2} + 3(\Delta n_0^2)^2 . \end{aligned} \quad (23)$$

Eq. (20) is self-evident, but Eq. (21) contains an important insight: Since $\langle n_\nu\rangle(\langle n_\nu\rangle + 1) = \Delta n_\nu^2$ is the fluctuation of the occupation number n_ν of the νth excited state ($\nu \geqslant 1$), Eq. (21) expresses the fact that in the condensate regime these occupation numbers are *uncorrelated* stochastic variables; one simply has to add up their variances to obtain the variance Δn_0^2 of the ground-state occupation number $n_0 = N - \sum_{\nu\geqslant 1} n_\nu$. This finding is a first hint that within the canonical ensemble there exist independent degrees of freedom in the condensate regime; this will become more clear from the "independent oscillator" point of view outlined in the following section.

3. Cumulants for the ideal Bose–Einstein condensate

The canonical condensate distribution (12), and the moments (14)–(17) derived from it, hinge on the validity of the quasithermal approximation (5). This ansatz appears quite reasonable, and it manifestly takes the constraint of fixed particle number into account, but its level of accuracy still needs to be quantified. In order to assess the accuracy of this quasithermal approximation, we will now tackle the problem of canonical condensate statistics from a different angle, staying strictly within the framework of orthodox equilibrium statistical mechanics, and trying to avoid any uncontrolled approximation. The price to pay for the mathematical rigor that will be attained in this and the following sections is that we have to remain restricted to temperatures below the onset of Bose–Einstein condensation, whereas the distribution (12) applies at all temperatures.

We start from the familiar representation [1–3]

$$Z_N(\beta) = {\sum_{\{n_\nu\}}}' \exp\left(-\beta\sum_\nu n_\nu\varepsilon_\nu\right) \tag{24}$$

of the canonical N-particle partition function, where the prime indicates that the summation runs only over those sets of occupation numbers $\{n_\nu\}$ that comply with the constraint $\sum_\nu n_\nu = N$. Singling out the ground-state energy $N\varepsilon_0$, we write the total energy of each such configuration as

$$\begin{aligned}\sum_\nu n_\nu\varepsilon_\nu &= \sum_\nu n_\nu(\varepsilon_\nu - \varepsilon_0) + N\varepsilon_0 \\ &\equiv E + N\varepsilon_0 ,\end{aligned} \tag{25}$$

so that E denotes the true excitation energy of the respective configuration. Grouping together configurations with identical excitation energies, we have

$$Z_N(\beta) = \sum_E \Omega(E,N)\exp(-\beta E - N\beta\varepsilon_0) , \tag{26}$$

with $\Omega(E,N)$ denoting the number of microstates accessible to an N-particle system with excitation energy E, that is, the number of microstates where E is distributed *over N or less* particles: $\Omega(E,N)$ counts all the configurations where E is concentrated on one particle only, or shared among two particles, or three, or any other number M up to N.

Detailed understanding of canonical (or microcanonical) statistics, however, requires knowledge of the number of microstates with *exactly* M excited particles, for all M up to N; these numbers are provided by the differences

$$\Phi(E,M) \equiv \Omega(E,M) - \Omega(E,M-1), \quad M = 0,1,2,\ldots,N . \tag{27}$$

By definition, $\Omega(E,-1) = 0$. Given $\Phi(E,M)$, the canonical probability distribution for finding M excited particles (and, hence, $N-M$ particles still residing in the ground state) at inverse temperature β is determined by

$$p_N^{(\mathrm{ex})}(M;\beta) \equiv \frac{\sum_E \mathrm{e}^{-\beta E}\Phi(E,M)}{\sum_E \mathrm{e}^{-\beta E}\Omega(E,N)}, \quad M = 0,1,2,\ldots,N . \tag{28}$$

This distribution is merely the mirror image of the condensate distribution p_{n_0} considered in the previous section, i.e., we have $p_N^{(\mathrm{ex})}(M;\beta) = p_{N-M}$. Since the definition (27) obviously implies

$$\sum_{M=0}^{N} \Phi(E,M) = \Omega(E,N) , \tag{29}$$

it is properly normalized,

$$\sum_{M=0}^{N} p_N^{(\mathrm{ex})}(M;\beta) = 1 . \tag{30}$$

In the following, we will derive a general formula which gives all cumulants of the canonical distribution (28), provided the temperature is so low that a significant fraction of the particles occupies the ground state—that is, provided there is a condensate.

To this end, we recall that the set of canonical M-particle partition functions $Z_M(\beta)$ is generated by the grand canonical partition function, which has a simple product form [1–3]:

$$\sum_{M=0}^{\infty} z^M Z_M(\beta) = \prod_{\nu=0}^{\infty} \frac{1}{1 - z\exp(-\beta\varepsilon_\nu)} , \tag{31}$$

here, z is a complex variable. However, every single M-particle partition function enters into this expression with its own, M-particle ground-state energy $M\varepsilon_0$. In order to remove these unwanted contributions, we define a slightly different function $\Xi(\beta,z)$ by multiplying each $Z_M(\beta)$ by $(z\mathrm{e}^{\beta\varepsilon_0})^M$, instead of z^M, and then summing over M, obtaining

$$\begin{aligned} \Xi(\beta,z) &\equiv \sum_{M=0}^{\infty} (z\mathrm{e}^{\beta\varepsilon_0})^M Z_M(\beta) \\ &= \prod_{\nu=0}^{\infty} \frac{1}{1 - z\,\exp[-\beta(\varepsilon_\nu - \varepsilon_0)]} . \end{aligned} \tag{32}$$

On the other hand, in view of Eq. (26) this function also has the representation

$$\Xi(\beta,z) = \sum_{M=0}^{\infty} z^M \sum_E \Omega(E,M)\,\exp(-\beta E)\,. \tag{33}$$

Therefore, multiplying $\Xi(\beta,z)$ by $1-z$ and suitably shifting the summation index M, we arrive at a generating function for the desired differences $\Phi(E,M)$:

$$\begin{aligned}(1-z)\Xi(\beta,z) &= \sum_{M=0}^{\infty}(z^M - z^{M+1})\sum_E \Omega(E,M)\,\exp(-\beta E) \\ &= \sum_{M=0}^{\infty} z^M \sum_E\,[\Omega(E,M) - \Omega(E,M-1)]\,\exp(-\beta E) \\ &= \sum_{M=0}^{\infty} z^M \sum_E \Phi(E,M)\,\exp(-\beta E)\,. \end{aligned} \tag{34}$$

Going back to the representation (32) now reveals that multiplying $\Xi(\beta,z)$ by $1-z$ means amputating the ground-state factor $v=0$ from this product and retaining only its "excited" part; we therefore denote the result as $\Xi_{\text{ex}}(\beta,z)$:

$$\begin{aligned}(1-z)\Xi(\beta,z) &= \prod_{v=1}^{\infty}\frac{1}{1 - z\,\exp[-\beta(\varepsilon_v - \varepsilon_0)]} \\ &\equiv \Xi_{\text{ex}}(\beta,z)\,. \end{aligned} \tag{35}$$

Moreover, from Eq. (34) it is obvious that the canonical moments of the unrestricted set $\Phi(E,M)$ (that is, the moments pertaining to *all* $\Phi(E,M)$ with $M \geqslant 0$) are obtained by repeatedly differentiating $\Xi_{\text{ex}}(\beta,z)$ with respect to z, and then setting $z=1$:

$$\left(z\frac{\partial}{\partial z}\right)^k \Xi_{\text{ex}}(\beta,z)\Bigg|_{z=1} = \sum_E\,\exp(-\beta E)\sum_{M=0}^{\infty} M^k\,\Phi(E,M)\,. \tag{36}$$

So far, all rearrangements have been exact.

For making contact with the actual N-particle system under consideration, we now have to restrict the summation index M: If the sum over M did not range over all particle numbers from zero to infinity, but rather were restricted to integers not exceeding the actual particle number N, then Eq. (36), together with the representation (35), would yield precisely the non-normalized kth moments of the canonical distribution (28). As it stands, however, exact equality is spoiled by the unrestricted summation. At this point, there is one crucial observation to be made: In the condensate regime the difference between the exact kth moment, given by a restricted sum, and the right-hand side of Eq. (36) must be exceedingly small [16]. Namely, if there is a condensate, then $\Phi(E,N)/\Omega(E,N)$ is negligible, since the statistical weight of those microstates with the energy E spread over all N particles must be insignificant—if it were not, so that there was a substantial probability for all N particles being excited, there would be no condensate! Consequently, we have $\Phi(E,M)/\Omega(E,N) \approx 0$ also for all M larger than

N: In the condensate regime it does not matter whether the upper limit of the sum over M in Eq. (36) is the actual particle number N, or infinity;

$$\sum_{M=0}^{\infty} M^k \Phi(E,M) \approx \sum_{M=0}^{N} M^k \Phi(E,M) \quad \text{in the condensate regime} . \tag{37}$$

Within this approximation—which will remain the only approximation in the entire argument!—the amputated function $\Xi_{\mathrm{ex}}(\beta,z)$ provides, by means of Eq. (36), the moments of the excited-states distribution (28), as long as one stays in the condensate regime.

The rationale behind this reasoning can be interpreted in a twofold manner. Intuitively, one may divide a partially condensed Bose gas into the excited-states subsystem, and a supply of condensate particles. The approximation (37) then means replacing the actual condensate, consisting of a finite number of particles, by an infinite particle reservoir [21]; this point of view goes back to Fierz [22]. Of course, the added condensate particles do not take part in the dynamics, so that the statistical properties of the excited subsystem remain unchanged. For our purposes, another interpretation is more telling: For $k=0$, and utilizing the representation (35) of the moment-generating function $\Xi_{\mathrm{ex}}(\beta,z)$, the approximation (37) brings Eq. (36) into the form

$$\begin{aligned}\prod_{\nu=1}^{\infty} \frac{1}{1-\exp[-\beta(\varepsilon_\nu-\varepsilon_0)]} &= \sum_E \exp(-\beta E) \sum_{M=0}^{N} \Phi(E,M) \\ &= \sum_E \exp(-\beta E)\Omega(E,N)\end{aligned} \tag{38}$$

—stating that in the condensate regime, where (37) holds, the canonical partition function of the Bose gas on the right-hand side equals that of a system of harmonic oscillators, with frequencies $\varepsilon_\nu - \varepsilon_0$ ($\nu \geqslant 1$), on the left-hand side of Eq. (38). While the original particles are indistinguishable, and subject to Bose statistics, the substituting oscillators obey Boltzmann statistics; the partition function of the oscillator system being the simple product of the geometric series representing the partition functions of the individual oscillators. It should be noted that this (almost-) isomorphism of a partially condensed, ideal Bose gas and a Boltzmannian harmonic oscillator system holds for any form of the single-particle spectrum, *not* only for harmonic traps.

Since, according to Eq. (36), the function $\Xi_{\mathrm{ex}}(\beta,z)$ generates the moments of the canonical distribution (28) in the condensate regime, its logarithm generates the cumulants $\kappa_k(\beta)$:

$$\kappa_k(\beta) = \left(z\frac{\partial}{\partial z}\right)^k \ln\, \Xi_{\mathrm{ex}}(\beta,z)\bigg|_{z=1} . \tag{39}$$

As is well known from elementary statistics, the kth order cumulant of the sum of independent stochastic variables is the sum of their individual kth order cumulants; moreover, all cumulants higher than the second vanish exactly for a Gaussian stochastic variable [23]. In the present case, taking the required derivatives of $\ln \Xi_{\mathrm{ex}}(\beta, z)$ and using expression (18) for the canonical occupation numbers $\langle n_\nu \rangle$ in the condensate regime, we find for $k = 1, \ldots, 4$:

$$\kappa_1(\beta) = \sum_{\nu \geqslant 1} \langle n_\nu \rangle \,, \tag{40}$$

$$\kappa_2(\beta) = \sum_{\nu \geqslant 1} \langle n_\nu \rangle (\langle n_\nu \rangle + 1) \,, \tag{41}$$

$$\kappa_3(\beta) = \sum_{\nu \geqslant 1} (\langle n_\nu \rangle + 3\langle n_\nu \rangle^2 + 2\langle n_\nu \rangle^3) \,, \tag{42}$$

$$\kappa_4(\beta) = \sum_{\nu \geqslant 1} (\langle n_\nu \rangle + 7\langle n_\nu \rangle^2 + 12\langle n_\nu \rangle^3 + 6\langle n_\nu \rangle^4) \,. \tag{43}$$

The fact that $\kappa_3(\beta)$ and $\kappa_4(\beta)$ are non-zero signals the non-Gaussian nature of the fluctuations; the fact that all cumulants are given as simple sums over the oscillator index ν reflects the independence of the individual Boltzmannian oscillators.

Because the excited-states distribution (28) is related to the ground-state distribution p_{n_0} through $p_{n_0} = p_N^{(\mathrm{ex})}(N - n_0; \beta)$, one also has

$$\begin{aligned} \kappa_1(\beta) &= N - \langle n_0 \rangle \,, \\ \kappa_2(\beta) &= \langle (n_0 - \langle n_0 \rangle)^2 \rangle \,, \\ \kappa_3(\beta) &= -\langle (n_0 - \langle n_0 \rangle)^3 \rangle \,, \\ \kappa_4(\beta) &= \langle (n_0 - \langle n_0 \rangle)^4 \rangle - 3\langle (n_0 - \langle n_0 \rangle)^2 \rangle^2 \,. \end{aligned} \tag{44}$$

Comparison of Eqs. (40)–(43) derived here from orthodox statistical mechanics with the previous master-equation results (20)–(23) thus shows that the master equation, solved within the quasithermal approximation (5), actually had yielded the first two cumulants exactly; the effect of the quasithermal approximation only consists in breaking higher-order moments into suitable combinations of first- and second-order ones:

$$\begin{aligned} \sum_{\nu \geqslant 1} \langle n_\nu \rangle^3 &\to \frac{(\sum_{\nu \geqslant 1} \langle n_\nu \rangle^2)^2}{\sum_{\nu \geqslant 1} \langle n_\nu \rangle} \,, \\ \sum_{\nu \geqslant 1} \langle n_\nu \rangle^4 &\to \frac{(\sum_{\nu \geqslant 1} \langle n_\nu \rangle^2)^3}{(\sum_{\nu \geqslant 1} \langle n_\nu \rangle)^2} \,. \end{aligned} \tag{45}$$

In this respect, the quasithermal approximation is a kind of mean field approximation.

For general $k \geqslant 1$, the cumulant $\kappa_k(\beta)$ is a linear combination of all moments of order lower than and equal to k:

$$\kappa_k(\beta) = \sum_{\nu \geqslant 1} \sum_{m=1}^{k} (m-1)! \sigma_k^{(m)} \langle n_\nu \rangle^m \,, \tag{46}$$

where $\sigma_k^{(m)}$ are the Stirling numbers of the second kind [18,24]; for $k = 1, \ldots, 4$, this formula (46) leads back to Eqs. (40)–(43). While it directly expresses the cumulants through the non-centered moments, Eq. (46) still leaves the cumbersome sums over v to be evaluated. In the following section, we will show how these summations can be circumvented by means of a Mellin–Barnes integral transformation.

4. Integral representation of the cumulant formula

We now exploit the representation (35) of the ground-state amputated function $\Xi_{\rm ex}(\beta,z)$ for writing the cumulant-generating function $\ln \Xi_{\rm ex}(\beta,z)$ in the form

$$\ln \Xi_{\rm ex}(\beta,z) = -\sum_{v=1}^{\infty} \ln(1 - z\exp[-\beta(\varepsilon_v - \varepsilon_0)]) = \sum_{v=1}^{\infty}\sum_{n=1}^{\infty} \frac{z^n \exp[-\beta(\varepsilon_v - \varepsilon_0)n]}{n}\,, \tag{47}$$

where we have made use of the series

$$\ln\,(1-x) = -\sum_{n=1}^{\infty} \frac{x^n}{n} \quad \text{for } -1 \leqslant x < 1\,. \tag{48}$$

Next, we employ the Mellin–Barnes integral representation [25]

$$e^{-a} = \frac{1}{2\pi i}\int_{\tau - i\infty}^{\tau + i\infty} dt\, a^{-t}\Gamma(t)\,, \tag{49}$$

valid for real $\tau > 0$ and complex numbers a with $\mathrm{Re}(a) > 0$, to arrive at

$$\ln \Xi_{\rm ex}(\beta,z) = \sum_{v=1}^{\infty}\sum_{n=1}^{\infty} \frac{1}{2\pi i}\int_{\tau - i\infty}^{\tau + i\infty} dt\,\Gamma(t)\,\frac{z^n}{n}\,\frac{1}{(\beta[\varepsilon_v - \varepsilon_0]n)^t} = \frac{1}{2\pi i}\int_{\tau - i\infty}^{\tau + i\infty} dt\,\Gamma(t)\sum_{v=1}^{\infty}\frac{1}{(\beta[\varepsilon_v - \varepsilon_0])^t}\sum_{n=1}^{\infty}\frac{z^n}{n^{t+1}}\,. \tag{50}$$

The last step, the interchange of summation and integration, is crucial; it requires that the sums be absolutely convergent. This, in turn, means that the real number τ has to be adjusted accordingly: The path of integration parallel to the imaginary axis of the complex t-plane has to lie on the right of all poles of the integrand.

Recalling now the series representation of the Bose functions $g_\alpha(z)$,

$$g_\alpha(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^\alpha}\,, \tag{51}$$

and introducing the generalized, "spectral" Zeta function [16]

$$Z(\beta,t) \equiv \sum_{v=1}^{\infty} \frac{1}{(\beta[\varepsilon_v - \varepsilon_0])^t}\,, \tag{52}$$

the formula (35) thus yields, without any approximation at all, the convenient integral representation

$$\ln \Xi_{\rm ex}(\beta,z) = \frac{1}{2\pi \mathrm{i}} \int_{\tau-\mathrm{i}\infty}^{\tau+\mathrm{i}\infty} \mathrm{d}t\, \Gamma(t) Z(\beta,t) g_{t+1}(z)\,. \tag{53}$$

The derivatives required by Eq. (39) for calculating the kth cumulant $\kappa_k(\beta)$ in the condensate regime now act only on the Bose function $g_{t+1}(z)$ appearing in the integrand. Utilizing the well-known relations

$$z\frac{\mathrm{d}}{\mathrm{d}z} g_\alpha(z) = g_{\alpha-1}(z) \tag{54}$$

and

$$g_\alpha(1) = \zeta(\alpha)\,, \tag{55}$$

where $\zeta(z)$ denotes the ordinary Riemann Zeta function, Eqs. (39) and (53) then lead directly to the appealingly compact formula

$$\kappa_k(\beta) = \frac{1}{2\pi \mathrm{i}} \int_{\tau-\mathrm{i}\infty}^{\tau+\mathrm{i}\infty} \mathrm{d}t\, \Gamma(t) Z(\beta,t) \zeta(t+1-k)\,. \tag{56}$$

This formula is a principal result of the present paper. By means of the residue theorem it links *all* the cumulants of the canonical distribution (28) in the condensate regime to the poles of the generalized Zeta function $Z(\beta,t)$, which embodies all the system's properties, and to the pole of a system-independent Riemann Zeta function, the location of which depends on the order k of the respective cumulant. Already at this point, an interesting competition becomes apparent: In the thermodynamic limit it is only the rightmost pole that matters, and this rightmost pole is provided *either* by $Z(\beta,t)$, *or* by $\zeta(t+1-k)$. Since the poles of $Z(\beta,t)$ do not depend on k, and that of $\zeta(t+1-k)$ lies at $t=k$, it is clear that for sufficiently large k it is always the Riemann function that determines the exponent of β, namely $\kappa_k(\beta) \propto \beta^{-k}$ for large k. It is only for low k, when the rightmost pole of $Z(\beta,t)$ takes over, that a particular system—that is, a particular type of trap—can mould exponents of its own.

5. Application to different traps

The usefulness of the cumulant formula (56) for practical purposes rests in the fact that there exist standard techniques for analytically continuing the generalized Zeta functions (52) to the complex t-plane; analytic continuation of the Riemann Zeta function $\zeta(t) = \sum_{n=1}^{\infty} n^{-t}$ is standard textbook knowledge [26]. Then the residues of the analytically continued integrands, taken from right to left, provide systematic asymptotic expansions of the cumulants $\kappa_k(\beta)$. In this section, we will exercise this program in detail for three different types of single-particle spectra, that is, for different types of trapping potentials.

5.1. The three-dimensional isotropic harmonic oscillator trap

In the case of an isotropic, three-dimensional harmonic oscillator potential with oscillator frequency ω, the single-particle energies read

$$\varepsilon_\nu = \hbar\omega(\nu + 1/2), \quad \nu = 0, 1, 2, \ldots\ ; \tag{57}$$

their degree of degeneracy is

$$g_\nu = \tfrac{1}{2}\nu^2 + \tfrac{3}{2}\nu + 1\ . \tag{58}$$

Therefore, the generalized Zeta function (52) reduces to a sum of Riemann Zeta functions and thus acquires a particularly simple form [16]:

$$\begin{aligned} Z(\beta,t) &= \sum_{\nu=1}^{\infty} \frac{g_\nu}{(\beta\hbar\omega\nu)^t} \\ &= (\beta\hbar\omega)^{-t}\left[\frac{1}{2}\zeta(t-2) + \frac{3}{2}\zeta(t-1) + \zeta(t)\right]\ . \end{aligned} \tag{59}$$

Hence, all we need to know is that $\zeta(z)$ possesses only one simple pole, located at $z = 1$ with residue $+1$, namely [26]

$$\zeta(z) \approx \frac{1}{z-1} + \gamma \quad \text{for } z \approx 1\ , \tag{60}$$

where $\gamma \approx 0.57722$ is Euler's constant. Because temperature enters into the cumulants (56) *only* via the prefactor $(\beta\hbar\omega)^{-t}$ of the spectral Zeta function (59), for temperatures T large compared to the level spacing temperature $\hbar\omega/k_B$ (that is, for $\beta\hbar\omega \ll 1$, so that the gas occupies more than just the lowest few trap states) the temperature dependence of the kth cumulant $\kappa_k(\beta)$ is governed by the factor $(\beta\hbar\omega)^{-p}$, where p is the position of the rightmost pole appearing in the integrand (56). Now $\Gamma(t)$ has poles at $t = 0, -1, -2, \ldots$, the spectral function (59) has poles at $t = 3, 2, 1$; and $\zeta(t+1-k)$ has a pole at $t = k$. Thus, for $k = 1, 2$ it is rightmost pole of the spectral Zeta function (59) that dominates, implying $\kappa_1(\beta) \propto (\beta\hbar\omega)^{-3}$ and $\kappa_2(\beta) \propto (\beta\hbar\omega)^{-3}$. For $k = 3$, the leading pole of $Z(\beta,t)$ at $t = 3$ coincides with the pole of $\zeta(t+1-k)$, so that $\kappa_3(\beta) \propto (\beta\hbar\omega)^{-3}$ with logarithmic corrections due to the double pole. For $k \geqslant 4$, the dominant pole is provided by $\zeta(t+1-k)$, giving $\kappa_k(\beta) \propto (\beta\hbar\omega)^{-k}$. Collecting also the next-to-leading poles, and computing the respective residues, we obtain the following asymptotic expressions, valid for $k_BT/(\hbar\omega) \gg 1$ in the condensate regime:

- The first cumulant $\kappa_1(\beta)$ of distribution (28) equals the canonical expectation value $\langle N_{\rm ex}\rangle$ of the number of excited particles. In the condensate regime, the expectation value $\langle n_0\rangle$ for the number of condensate particles is then given by $N - \langle N_{\rm ex}\rangle = N - \kappa_1(\beta)$:

$$\langle n_0\rangle \sim N - \left(\frac{k_BT}{\hbar\omega}\right)^3 \zeta(3) - \left(\frac{k_BT}{\hbar\omega}\right)^2 \frac{3}{2}\zeta(2) - \frac{k_BT}{\hbar\omega}\left[\ln\left(\frac{k_BT}{\hbar\omega}\right) + \gamma - \frac{19}{24}\right]\ , \tag{61}$$

where we have taken into account the three poles at $t = 3, 2, 1$; the logarithm in the last term stems from the double pole at $t = 1$.

- The second cumulant $\kappa_2(\beta)$ yields the mean-square fluctuation of the number of excited particles. Since the total particle number N is constant, this equals the mean-square fluctuation of the number of condensate particles, $\kappa_2(\beta) = \Delta N_{\rm ex}^2 = \Delta n_0^2$. To the same accuracy as Eq. (61), we find

$$\Delta n_0^2 \sim \left(\frac{k_B T}{\hbar\omega}\right)^3 \zeta(2) + \left(\frac{k_B T}{\hbar\omega}\right)^2 \left[\frac{3}{2}\ln\left(\frac{k_B T}{\hbar\omega}\right) + \frac{3}{2}\gamma + \frac{5}{4} + \zeta(2)\right] + \frac{k_B T}{\hbar\omega}\left(-\frac{1}{2}\right) ; \tag{62}$$

the double pole now appearing at $t = 2$ in the integrand (56). The leading term here agrees with the result first stated by Politzer [27], but obviously the corrections to this term are quite significant for finite, moderate N.

- The third cumulant equals the third central moment, implying $\kappa_3(\beta) = \langle (N_{\rm ex} - \langle N_{\rm ex}\rangle)^3\rangle = -\langle (n_0 - \langle n_0\rangle)^3\rangle$. Therefore,

$$\langle (n_0 - \langle n_0\rangle)^3\rangle \sim -\left(\frac{k_B T}{\hbar\omega}\right)^3 \left[\ln\left(\frac{k_B T}{\hbar\omega}\right) + \gamma + \frac{3}{2} + 3\zeta(2) + 2\zeta(3)\right] + \left(\frac{k_B T}{\hbar\omega}\right)^2 \frac{3}{4} + \frac{k_B T}{\hbar\omega}\frac{1}{12} . \tag{63}$$

- The calculation of all higher cumulants is even simpler, since there are no more double poles and, consequently, no more logarithmic corrections like those in Eqs. (61)–(63). For example, the fourth cumulant, related to the fourth central moment by $\kappa_4(\beta) = \langle (n_0 - \langle n_0\rangle)^4\rangle - 3\kappa_2(\beta)^2$, turns out to be

$$\kappa_4(\beta) \sim \left(\frac{k_B T}{\hbar\omega}\right)^4 [3\zeta(2) + 9\zeta(3) + 6\zeta(4)] + \left(\frac{k_B T}{\hbar\omega}\right)^3 \left(-\frac{1}{2}\right) + \left(\frac{k_B T}{\hbar\omega}\right)^2 \left(-\frac{1}{8}\right) . \tag{64}$$

It is an elementary fact that for some given distribution either all cumulants higher than the second vanish—in which case the distribution is Gaussian—or that there are infinitely many non-vanishing cumulants [23]. Therefore, the distribution (28), which describes the number of excited particles in a partially condensed ideal Bose gas, is non-Gaussian; the deviations from a Gaussian distribution being quantified by the magnitude of $\kappa_k(\beta)$, $k \geqslant 3$. It should be noted that the above results are *independent* of the particle number N, so that one does not recover a Gaussian distribution in the (unphysical) limit $N \to \infty$, when ω and T are held constant.

For checking these asymptotic formulae, we resort to the familiar recursion relation [28,29]

$$Z_N(\beta) = \frac{1}{N}\sum_{k=1}^{N} Z_1(k\beta) Z_{N-k}(\beta), \quad Z_0(\beta) \equiv 1 , \tag{65}$$

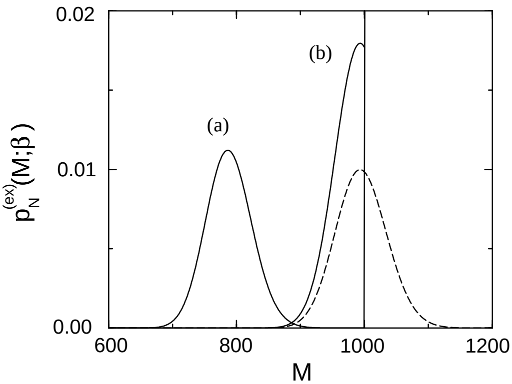

Fig. 2. Exact distributions $p_N^{(\mathrm{ex})}(M;\beta)$ for $N=1000$ particles in a three-dimensional harmonic oscillator trap: Curve (a) corresponds to $k_BT/(\hbar\omega)=8.0$, lower than the onset of Bose–Einstein condensation. In this case, the distribution has no appreciable weight at the maximum argument $M=1000$, so that the approximation (37) is safe. Curve (b) corresponds to a temperature in the transition regime, $k_BT/(\hbar\omega)=8.7$. Since the number M of excited particles cannot exceed the total particle number N, the exact distribution now is strongly asymmetric. The approximation (37), ignoring this restriction, would yield the dashed distribution.

which allows us to obtain the exact canonical partition functions at least numerically. The canonical probability for finding n out of the N particles in the αth excited state then follows from [30]

$$P_\alpha(n|N)=\exp(-\beta\varepsilon_\alpha n)\frac{Z_{N-n}(\beta)}{Z_N(\beta)}-\exp[-\beta\varepsilon_\alpha(n+1)]\frac{Z_{N-n-1}(\beta)}{Z_N(\beta)}\,. \tag{66}$$

Specializing $\alpha=0$ gives the ground-state occupation probability p_{n_0} as considered in Section 2; $p_{n_0}=p_N^{(\mathrm{ex})}(N-n_0;\beta)=P_0(n_0|N)$.

We use these relations first for visualizing the content of the key approximation (37): Fig. 2 shows the exact distribution $p_N^{(\mathrm{ex})}(M;\beta)$ for $N=1000$ particles in a three-dimensional isotropic harmonic oscillator trap with $k_BT/(\hbar\omega)=8.0$, a temperature well below the onset of Bose–Einstein condensation. In this case, the expected number of excited particles is roughly 800; the distribution decays so rapidly towards higher M that its tail contains no appreciable weight when reaching the largest possible value, $M_{\max}=N=1000$. Therefore, it would remain practically unchanged—so that approximation (37) is entirely safe—if the particle number N were increased to any higher value, or even to infinity, as it happens when adopting approximation (37). This is what effectuates the N-independence of the condensate's statistical properties, as met in Eqs. (62)–(64). The situation is different, however, for $k_BT/(\hbar\omega)=8.7$, a temperature in the transition regime: On the average, almost all particles are excited then. Since it is obviously impossible to excite more than the available N particles, the exact distribution now becomes highly asymmetric. Approximation (37), on the other hand, assumes an infinite supply of condensate particles and thus ignores the restriction

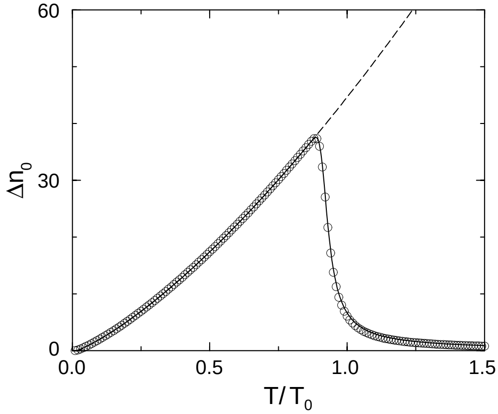

Fig. 3. Root-mean-square fluctuation $\Delta n_0 = (\Delta n_0^2)^{1/2}$ for $N = 1000$ particles in a three-dimensional harmonic oscillator trap. The full line is the result provided by the solution of the master equation within the quasithermal approximation, circles indicate exact numerical data, and the dashed line is the prediction made by the cumulant formula (56).

$M \leqslant N$; in the present example, the distribution implied by this approximation would be correct only if the total particle number were larger than about 1200. In general, the approximation (37) remains reliable just as long as the support of the distribution $p_N^{(\mathrm{ex})}(M;\beta)$ stays away from the "wall" at $M = N$, and in this way remains insensitive to the magnitude of N. In short, one requires

$$\langle (n_0 - \langle n_0 \rangle)^2 \rangle^{1/2} \ll \langle n_0 \rangle \; . \tag{67}$$

Fig. 3 depicts the r.m.s.-fluctuation $\Delta n_0 \equiv (\Delta n_0^2)^{1/2}$ of the number of condensate particles, again for $N = 1000$ Bosons in an isotropic harmonic trap. In this and all following figures, the full line indicates the result obtained from solution (12) to the master equation (4)—which embodies the quasithermal approximation (5)—circles correspond to exact numerical data calculated with the help of the recursion relation (65), and the dashed line is the prediction of the asymptotic approximation (62) to the cumulant formula (56). Temperature is scaled with respect to the characteristic temperature

$$T_0 = \frac{\hbar\omega}{k_B}\left(\frac{N}{\zeta(3)}\right)^{1/3} \tag{68}$$

which marks the Bose–Einstein transition temperature for rather large N [31]; T_0 is obtained formally by setting $\langle n_0 \rangle = 0$ in Eq. (61) and ignoring all temperature-dependent terms except for the leading, T^3-proportional one. For the relatively small number $N = 1000$ considered here, this furnishes only a rough approximation to the actual transition temperature (which, of course, is not a sharply defined quantity in finite systems), since the neglected next-to-leading term amounts to a reduction of the ground-state

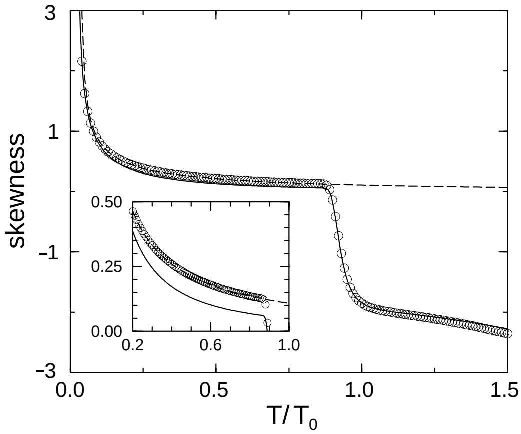

Fig. 4. Skewness $\kappa_3(\beta)/\kappa_2(\beta)^{3/2}$ for $N = 1000$ particles in a three-dimensional harmonic oscillator trap. The symbols have the same meaning as in Fig. 3. The inset emphasizes that the cumulant formula (56) provides a perfect description of the exact data in the condensate regime, as expected. Note that the dashed line approaches the Gaussian value 0.

population. Therefore, keeping this term gives a downward shift of the transition temperature [32,33],

$$\frac{\Delta T_0}{T_0} = -\frac{\zeta(2)}{2\zeta(3)^{2/3}}\frac{1}{N^{1/3}} ; \tag{69}$$

this shift is in good agreement with the numerical data. For $N = 1000$ one finds $\Delta T_0 \approx -0.073T_0$, locating the transition at about $0.93T_0$; the maximum of the exact fluctuation data is found at $0.89T_0$. As witnessed by Fig. 3, in the condensate regime there is perfect agreement of all three data sets. This, of course, is only to be expected: The condensate regime corresponds to distributions of the type (a) in Fig. 2, so that approximation (37) has almost no effect and the cumulant formula (56), or its elementary, equivalent precursor (39) is practically exact. As noted before, for $k = 2$ the "oscillator" viewpoint leads to the same result as the master equation approach; Eq. (41) equals Eq. (21). What could not be expected, though, is that the master equation leads to excellent agreement with the exact fluctuation data for *all* temperatures, whereas the cumulant formula, by its very construction, is invalid for temperatures above T_0: In that regime it provides the curve which the exact data *would* follow if the number of particles were increased.

In contrast to the orders $k = 1, 2$, the calculation of the higher cumulants constitutes a non-trivial test of the master equation in the condensate regime. To this end, Fig. 4 shows the skewness (that is, the asymmetry coefficient) $\kappa_3(\beta)/\kappa_2(\beta)^{3/2}$, and Fig. 5 depicts the flatness $\kappa_4(\beta)/\kappa_2(\beta)^2 + 3$ (the excess coefficient, which equals the ratio of the fourth central moment to the square of the second central moment). The master equation does quite well for the skewness, underestimating the exact data just slightly in the condensate regime—where, of course, the cumulant formula (56) yields

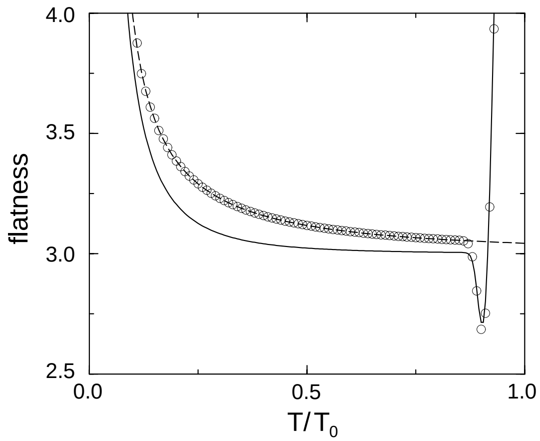

Fig. 5. Flatness $\kappa_4(\beta)/\kappa_2(\beta)^2 + 3$ for $N = 1000$ particles in a three-dimensional harmonic oscillator trap. The symbols have the same meaning as in Fig. 3. Note that the dashed line approaches the Gaussian value 3.

perfect agreement—but then actually locks on to the exact data above T_0. The same tendency is observed in Fig. 5: The master equation data underestimate the true flatness in the condensate regime, but are fairly accurate for higher temperatures.

It is also of interest to investigate the behavior of the cumulants in the large-system limit [7]. Since merely increasing the particle number N in a trap with fixed oscillator frequency ω would be accompanied by an unlimited increase of the characteristic temperature (68), we stipulate that, while N increases, ω be decreased proportionally to $N^{-1/3}$, so that T_0 stays constant. Substituting

$$\frac{k_B T}{\hbar\omega} = \frac{T}{T_0}\left(\frac{N}{\zeta(3)}\right)^{1/3} , \tag{70}$$

Eqs. (62)–(64) immediately show that in the condensate regime both skewness and flatness adopt precisely the Gaussian values in this limit,

$$\begin{aligned} &\frac{\kappa_3(\beta)}{\kappa_2(\beta)^{3/2}} \to 0 \\ &\frac{\kappa_4(\beta)}{\kappa_2(\beta)^2} + 3 \to 3, \quad T/T_0 \text{ fixed} . \end{aligned} \tag{71}$$

This recovery of Gaussian properties for “large” oscillator traps has already been hinted at by the dashed lines in Figs. 4 and 5, through their approach to the Gaussian values at high temperatures. But this does *not* mean that one is always left with Gaussian condensate fluctuations for sufficiently large systems; the following two examples will reveal that, and elucidate why, the cumulants can even retain a sensitivity to the boundary conditions in the thermodynamic limit.

5.2. The three-dimensional box with periodic boundary conditions

An ideal Bose gas confined to a cubic volume $V = L^3$ with periodic boundary conditions imposed on the wave functions is a somewhat artificial model system, if one is thinking of a mesoscopic sample of Bosonic atoms stored in a magnetic trap, but it is this model which is traditionally used in textbook treatments of the ideal Bose gas [1–3]. We write its single-particle energies as

$$\begin{aligned} \varepsilon_{n_1,n_2,n_3} &= \frac{\hbar^2(2\pi)^2}{2mL^2}(n_1^2 + n_2^2 + n_3^2) \\ &\equiv \hbar\Omega(n_1^2 + n_2^2 + n_3^2) \quad \text{with } n_\nu = 0, \pm 1, \pm 2 \pm \cdots , \end{aligned} \tag{72}$$

where m is the particle mass, and we have introduced the characteristic frequency

$$\Omega = \frac{\hbar(2\pi)^2}{2mL^2} . \tag{73}$$

Therefore, the spectral Zeta function now becomes

$$\begin{aligned} Z(\beta, t) &= (\beta\hbar\Omega)^{-t} \sum_{n_1,\,n_2,\,n_3=-\infty}^{+\infty}{}' \frac{1}{(n_1^2 + n_2^2 + n_3^2)^t} \\ &\equiv (\beta\hbar\Omega)^{-t} S(t) \end{aligned} \tag{74}$$

the prime indicating that, according to the general recipe (52), the ground state $(n_1, n_2, n_3) = (0, 0, 0)$ has to be omitted from the sum $S(t)$. Rewriting this sum such that only positive indices occur, it can be expressed as

$$S(t) = 8E_3(t) + 12E_2(t) + 6E_1(t) , \tag{75}$$

where

$$E_d(t) \equiv \sum_{n_1,\ldots,n_d=1}^{\infty} (n_1^2 + \ldots + n_d^2)^{-t} \tag{76}$$

is a d-dimensional Epstein Zeta function [34]; obviously, we have $E_1(t) = \zeta(2t)$. The three terms on the right-hand side of Eq. (75) reflect, respectively, the contributions from the eight octants in the space of all triples (n_1, n_2, n_3) where all three indices n_ν are non-vanishing, from the twelve quarter-planes with one vanishing index, and from the six half-lines where two indices are zero. Adding up the residues of these Epstein functions, as obtained in Eqs. (A.11), (A.13), and (A.15) of Appendix A, we find that $S(t)$ has merely one simple pole at

$$t = \tfrac{3}{2} \quad \text{with residue } 2\pi ; \tag{77}$$

the additional poles provided by $E_3(t)$, $E_2(t)$ and $E_1(t)$ at $t = 1$ and $t = \frac{1}{2}$ cancel exactly in the sum $S(t)$. This is no accident: Since the single-particle energies are determined by the spectrum of the Laplacian, the pole structure of $Z(\beta, t)$ encodes, in a sense, the geometry of the underlying domain; but for a simple cube with periodic boundary conditions there is not much to encode. In any case, this knowledge (77), together with the pole structure (60) of the Riemann Zeta function, is all that is required for evaluating the cumulant formula (56):

- For $k=1$, the pole of $S(t)$ at $t=\frac{3}{2}$ lies to the right of the pole placed by $\zeta(t+1-k)$ at $t=1$. Therefore, the canonical expectation value $\langle n_0\rangle = N-\kappa_1(\beta)$ for the number of condensate particles becomes

$$\begin{aligned}\langle n_0\rangle &\sim N-\Gamma(3/2)(\beta\hbar\Omega)^{-3/2}\,2\pi\,\zeta(3/2)-(\beta\hbar\Omega)^{-1}S(1)\\ &= N-\pi^{3/2}\zeta(3/2)\left(\frac{k_BT}{\hbar\Omega}\right)^{3/2}-S(1)\,\frac{k_BT}{\hbar\Omega}\,. \end{aligned}\tag{78}$$

  Inserting definition (73) of the frequency Ω, writing the periodicity volume as $V=L^3$, and using the thermal wavelength

$$\lambda_T=\frac{2\pi\hbar}{\sqrt{2\pi m k_BT}}\;;\tag{79}$$

  this Eq. (78) can be recast in the form

$$\langle n_0\rangle \sim N-\zeta(3/2)\frac{V}{\lambda_T^3}-S(1)\frac{V^{2/3}}{\pi\lambda_T^2}\,.\tag{80}$$

  In the thermodynamic limit (that is, for $N\to\infty$ and $V\to\infty$, such that the density N/V remains constant) the last term on the right-hand side may be neglected. Then one recovers a familiar textbook expression for the number of condensate particles, usually derived within the grand canonical ensemble [1–3], instead of the canonical ensemble employed here. It is valid as long as $\langle n_0\rangle>0$; the equation $\langle n_0\rangle=0$ defines the condensation temperature T_0: In the thermodynamic limit, one has

$$T_0=\frac{\hbar\Omega}{\pi k_B}\left(\frac{N}{\zeta(3/2)}\right)^{2/3}\;;\tag{81}$$

  for finite systems, where the additional term in Eq. (78) effectively increases the ground state occupation number (—observe that $S(1)\approx-8.9136$ is *negative*—), the transition temperature is minutely shifted upward.
- For $k\geqslant 2$ the situation is reversed: Now the pole of $\zeta(t+1-k)$ at $t=k$ lies to the right of its rival (77), giving

$$\kappa_k(\beta)\sim(k-1)!S(k)\left(\frac{k_BT}{\hbar\Omega}\right)^{k}+\pi^{3/2}\zeta(5/2-k)\left(\frac{k_BT}{\hbar\Omega}\right)^{3/2}\,.\tag{82}$$

  Specializing this latter result (82) to $k=2$, and inserting the numerical value $S(2)=8E_3(2)+12E_2(2)+6\zeta(4)\approx 16.532$ together with $\zeta(1/2)\approx-1.4604$, we find the condensate fluctuations

$$\Delta n_0^2\approx 16.532\left(\frac{k_BT}{\hbar\Omega}\right)^{2}-8.132\left(\frac{k_BT}{\hbar\Omega}\right)^{3/2}\,.\tag{83}$$

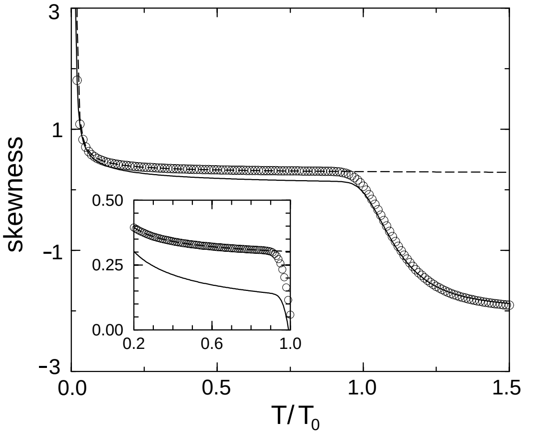

Fig. 6. Skewness $\kappa_3(\beta)/\kappa_2(\beta)^{3/2}$ for $N = 1000$ particles in a "box" trap with periodic boundary conditions. The symbols have the same meaning as in Fig. 3. Note that, in contrast to Fig. 4, the dashed line does not approach the Gaussian value 0, but rather 0.25.

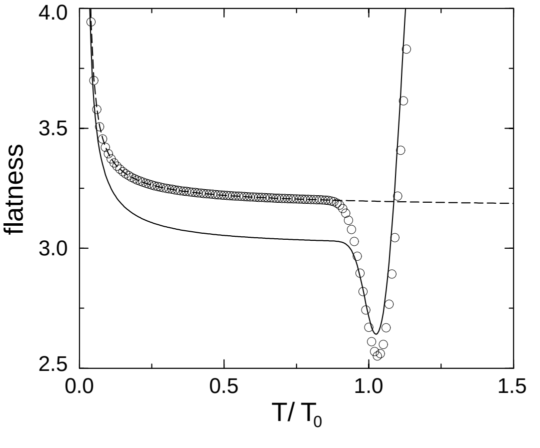

Fig. 7. Flatness $\kappa_4(\beta)/\kappa_2(\beta)^2 + 3$ for $N = 1000$ particles in a "box" trap with periodic boundary conditions. The symbols have the same meaning as in Fig. 3. Note that, in contrast to Fig. 5, the dashed line does not approach the Gaussian value 3, but rather 3.1525.

The Figs. 6 and 7 show, respectively, skewness and flatness of the excited-particles distribution (28) for $N = 1000$ ideal Bosons in a "box" trap with periodic boundary conditions; the reference temperature being given by Eq. (81). As before, exact data are compared to the predictions made by the master equation and the cumulant formula. Qualitatively, these figures resemble the previous Figs. 4 and 5 for the oscillator trap: The master equation data slightly underestimate skewness and flatness in the condensate regime, but fit surprisingly well for higher temperatures; the asymptotic expressions derived from the cumulant formula yield perfect agreement in the condensate regime.

There is, however, an important difference: As follows from Eq. (82), the dashed lines do not approach the Gaussian values at high temperatures; rather, the limit of skewness is 0.2500; the limit of flatness turns out to be 3.1525. The same values also characterize the thermodynamic limit:

$$\frac{\kappa_3(\beta)}{\kappa_2(\beta)^{3/2}} \to 0.2500\,,$$

$$\frac{\kappa_4(\beta)}{\kappa_2(\beta)^2} + 3 \to 3.1525; \quad N \to \infty, \quad V \to \infty, \quad N/V = \text{const}\,. \tag{84}$$

Thus, in contrast to the oscillator trap, the condensate fluctuations remain non-Gaussian even when the system becomes infinitely large [7]. We postpone a discussion of this finding to the next subsection, in order to emphasize its dependence on the boundary conditions.

5.3. The three-dimensional box with hard walls

If the N-particle Bose gas is stored in a cube $V = L^3$ with impenetrable walls, which from the physical viewpoint might be a more realistic assumption than that of periodic boundary conditions, we have to replace the former boundary conditions by Dirichlet ones, that is, the wave functions have to vanish at the walls of the container. This requirement yields the single-particle spectrum

$$\varepsilon_{n_1,n_2,n_3} = \tfrac{1}{4}\hbar\Omega(n_1^2 + n_2^2 + n_3^2) \quad \text{with } n_\nu = 1, 2, 3, \ldots\,, \tag{85}$$

with Ω as defined in Eq. (73). Compared with spectrum (72) for periodic boundary conditions, the level spacings now are reduced, as expressed by the prefactor $\frac{1}{4}$, but the quantum numbers n_ν comprise positive integers only, to the effect that the respective leading terms of the two densities of states $\rho(\varepsilon)$ coincide, in accordance with Weyl's celebrated theorem on the asymptotics of the spectrum of the Laplacian [35,36]. Therefore, in the thermodynamic limit all those quantities that can be evaluated with the help of the density of states do not depend on the respective boundary conditions. This applies, in particular, to the condensation temperature, or (what amounts to the same thing) to the first cumulant $\kappa_1(\beta)$. Namely, following London's classic work [37] we may approximate

$$\sum_{\nu \geqslant 1} \frac{1}{\exp[\beta(\varepsilon_\nu - \varepsilon_0)] - 1} \approx \int_0^\infty \frac{\rho(\varepsilon)\,\mathrm{d}\varepsilon}{\exp(\beta\varepsilon) - 1}\,, \tag{86}$$

with the density $\rho(\varepsilon)$ adapted to the boundary condition under study; in the thermodynamic limit the boundary-condition independence of the leading term of $\rho(\varepsilon)$ then implies the boundary-condition independence of $\kappa_1(\beta)$.

However, when dealing with a box potential this continuous-spectrum approximation ceases to work already for sum (41) which gives the second cumulant $\kappa_2(\beta)$, because the emerging integral is formally infrared-divergent [7]. Such a divergence occurs also for all higher cumulants; it is reflected by the fact that the rightmost pole in the cumulant formula (56) is that of $\zeta(t+1-k)$. Then Weyl's theorem cannot be invoked, so that there is *no* reason at all to assume that the boundary-condition independence of the first cumulant (in the thermodynamic limit) also extends to the higher cumulants. The study of the influence of the boundary conditions on these "higher" statistical properties, for which the cumulant formula (56) furnishes a most valuable tool, is thus a non-trivial enterprise.

The generalized Zeta function (52) associated with the spectrum (85) takes the form

$$\begin{aligned} Z(\beta,t) &= \left(\frac{1}{4}\beta\hbar\Omega\right)^{-t} \sum_{n_1,n_2,n_3=1}^{\infty}{}' \frac{1}{(n_1^2+n_2^2+n_3^2-3)^t} \\ &\equiv \left(\frac{1}{4}\beta\hbar\Omega\right)^{-t} \tilde{S}(t)\,, \end{aligned} \tag{87}$$

with the ground-state triple $(n_1,n_2,n_3)=(1,1,1)$ being excluded from the sum $\tilde{S}(t)$. As opposed to the case of periodic boundary conditions, subtraction of the non-zero ground-state energy now results in an *inhomogeneous* Zeta function. Paralleling the reasoning behind the arrangement (75), we disentangle those contributions where none, or one, or two of the indices n_ν equal 1, and write

$$\tilde{S}(t) = \tilde{E}_3(t) + 3\tilde{E}_2(t) + 3\tilde{E}_1(t)\,, \tag{88}$$

with inhomogeneous d-dimensional Epstein functions [34]

$$\tilde{E}_d(t) \equiv \sum_{n_1,\ldots,n_d=2}^{\infty} (n_1^2+\cdots+n_d^2-d)^{-t}\,. \tag{89}$$

Note that all indices of summation now start only at $n_\nu = 2$. Adding the residues found in Eqs. (A.19), (A.21), and (A.23) with the proper weights, one sees that the leading three poles of $\tilde{S}(t)$ reside at

$$t = 3/2, 1, 1/2 \quad \text{with residues } \frac{\pi}{4}, -\frac{3\pi}{8}, \frac{3+3\pi}{8}\,; \tag{90}$$

further poles at negative half-integer t will be neglected. With this input, the cumulant formula (56) can be set to work:

- For $k=1$, we encounter simple poles at $t=\frac{3}{2}$ and $t=\frac{1}{2}$, together with a double pole at $t=1$. Therefore, we also need the finite part δ of $\tilde{S}(t)$ at $t=1$, which plays the same role as Euler's constant γ did in Eq. (60):

$$\tilde{S}(t) \approx -\frac{3\pi/8}{t-1} + \delta \quad \text{for } t \approx 1\,. \tag{91}$$

The number of condensate particles, $\langle n_0\rangle = N - \kappa_1(\beta)$, is then found to be

$$\begin{aligned} \langle n_0\rangle \sim N &- \pi^{3/2}\zeta(3/2)\left(\frac{k_BT}{\hbar\Omega}\right)^{3/2} + \left[\frac{3\pi}{2}\ln\left(\frac{4k_BT}{\hbar\Omega}\right) - 4\delta\right]\frac{k_BT}{\hbar\omega} \\ &- \frac{3}{4}(1+\pi)\sqrt{\pi}\zeta(1/2)\left(\frac{k_BT}{\hbar\Omega}\right)^{1/2}\,. \end{aligned} \tag{92}$$

- For $k \geqslant 2$ there are simple poles at $t = k, \frac{3}{2}, 1, \frac{1}{2}$. Thus, the evaluation of the cumulant formula (56) is merely a matter of routine:

$$\kappa_k(\beta) \sim 4^k(k-1)!\,\tilde{S}(k)\left(\frac{k_BT}{\hbar\Omega}\right)^k + \pi^{3/2}\zeta(5/2-k)\left(\frac{k_BT}{\hbar\Omega}\right)^{3/2}$$
$$-\frac{3\pi}{2}\zeta(2-k)\frac{k_BT}{\hbar\Omega} + \frac{3}{4}(1+\pi)\sqrt{\pi}\zeta(3/2-k)\left(\frac{k_BT}{\hbar\Omega}\right)^{1/2} . \qquad (93)$$

It is worthwhile to discuss these results in some detail. To begin with, the ground-state occupation number (92) in a box with hard walls is logarithmically enhanced over the corresponding expression (78) for periodic boundary conditions. The reason for this enhancement derives from the observation that the quantum numbers n_ν range from $-\infty$ to $+\infty$ for periodic boundary conditions, see Eq. (72), whereas they are restricted to strictly positive integers in the hard-wall case, as stated in Eq. (85). Obviously one does *not* obtain the equivalent of *all* triples (n_1, n_2, n_3), with $-\infty \leqslant n_\nu \leqslant +\infty$, by taking eight times the octant of triples with strictly positive entries, since the planes with at least one of the n_ν equal to zero are still missing then. Hence, compared to the case of the periodic box, the density of states $\rho(\varepsilon)$ for Dirichlet boundary conditions is slightly reduced. This reduction does not concern the leading "volume" term of $\rho(\varepsilon)$, but merely constitutes a "surface" correction [35,36]. Thus, at low temperatures there are slightly less states accessible in a hard box than there would be in a hypothetical, same-sized box with periodic boundary conditions. This lack of states results in an enlarged ground state occupation number, so that Bose–Einstein condensation in a hard box sets in already at a higher temperature than it would in the periodic case [38]. Since the reduction of the density of states is not a leading-order effect, both condensation temperatures still agree in the thermodynamic limit, as already anticipated, and as clearly borne out by Eqs. (78) and (92): In the large-volume limit, where Ω becomes arbitrarily small, so that $k_BT/(\hbar\Omega)$ becomes very large even in the condensate regime, the logarithmic enhancement of $\langle n_0 \rangle$ in Eq. (92) remains hidden behind the $T^{3/2}$-proportional term. Our cumulant formula (56) expresses this asymptotic equality of both cumulants $\kappa_1(\beta)$ by means of its asymptotic sensitivity to only the rightmost pole. For $k = 1$, this is the pole of $Z(\beta, t)$ at $t = \frac{3}{2}$, with $Z(\beta, t)$ being given by either Eq. (74) or Eq. (87); asymptotic equality becomes visible through the fact that the residue (77) for the periodic box is just eight times the leading residue in Eq. (90) for its Dirichlet counterpart, corresponding to the eight octants of triples.

In contrast, for $k \geqslant 2$ the rightmost pole in Eq. (56) is no longer provided by the spectral Zeta function $Z(\beta, t)$, but rather by $\zeta(t+1-k)$, so that $Z(\beta, t)$ does not enter, to leading order, through its residue, but through its very value $Z(\beta, k)$ instead. Consequently, the "missing states" make themselves felt regardless of the system size: $4^k\tilde{S}(k)$ is not equal to $S(k)$, which means that *all higher cumulants* (82) *for the periodic box do not agree with their counterparts* (93) *for the Dirichlet box even in the thermodynamic limit.* Taking $k = 2$, for instance, we had found $S(2) \approx 16.532$ in

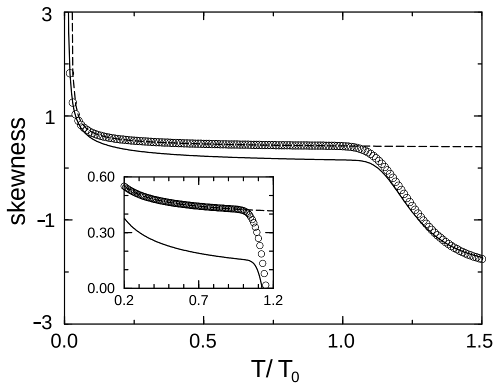

Fig. 8. Skewness $\kappa_3(\beta)/\kappa_2(\beta)^{3/2}$ for $N = 1000$ particles in a "box" trap with hard walls. The symbols have the same meaning as in Fig. 3. The dashed line approaches the value 0.3445, substantially higher than the limit attained with periodic boundary conditions in Fig. 6. Observe that the scale of the inset here differs from that in Fig. 6.

Eq. (83), whereas $16\,\tilde{S}(2) \approx 14.297$, so that Eq. (93) becomes

$$\Delta n_0^2 \approx 14.297 \left(\frac{k_B T}{\hbar\Omega}\right)^2 - 8.132 \left(\frac{k_B T}{\hbar\Omega}\right)^{3/2} + 2.356 \frac{k_B T}{\hbar\Omega} - 1.145 \left(\frac{k_B T}{\hbar\Omega}\right)^{1/2} . \tag{94}$$

Even in the thermodynamic limit, where only the leading term matters, the mean-square fluctuation of the number of condensate particles in a Dirichlet box is by 13.5% smaller than in a fictitious box with periodic boundary conditions.

Confirmation of these analytical deductions is drawn from Figs. 8 and 9, which quantify skewness and flatness of the distribution (28) for $N = 1000$ particles in a hard-walled box; in both cases the dashed line, drawn on the basis of the approximation (93), fully captures the exact non-Gaussian condensate statistics. The upward shift of the condensation temperature, as compared to periodic boundary conditions, is evident when juxtaposing these figures with the previous Figs. 6 and 7. Whereas this shift vanishes in the thermodynamic limit, another difference persists: As follows immediately from Eq. (93), skewness and flatness do not approach the values (84) here, but rather the substantially higher limits

$$\frac{\kappa_3(\beta)}{\kappa_2(\beta)^{3/2}} \to 0.3445 ,$$

$$\frac{\kappa_4(\beta)}{\kappa_2(\beta)^2} + 3 \to 3.3084; \quad N \to \infty, \quad V \to \infty, \quad N/V = \text{const} . \tag{95}$$

The mechanism sustaining this boundary-condition dependence even in the thermodynamic limit is, of course, the same as discussed before for the fluctuations; when the density of states cannot be invoked for converting sums like that in Eq. (41) into

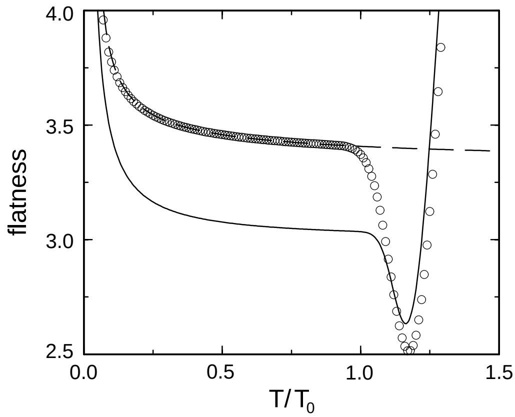

Fig. 9. Flatness $\kappa_4(\beta)/\kappa_2(\beta)^2 + 3$ for $N = 1000$ particles in a "box" trap with hard walls. The symbols have the same meaning as in Fig. 3. The dashed line approaches the value 3.3084, substantially higher than the limit attained with periodic boundary conditions in Fig. 7.

integrals, because the integrals would be infrared-divergent, Weyl's theorem does not come into play.

6. Discussion

The fluctuation of the number of condensate particles in an ideal Bose gas depends on the statistical ensemble involved: The large fluctuations arising in the grand canonical ensemble, $\Delta n_0^2 = \langle n_0\rangle(\langle n_0\rangle + 1)$, in a canonical setting give way to much smaller fluctuations $\Delta n_0^2 = \sum_{v\geqslant 1} \langle n_v\rangle \; (\langle n_v\rangle + 1)$, i.e., when there is no exchange of particles with a reservoir, and they are reduced still further under microcanonical conditions [14,16,21], when the system is also thermally isolated from its environment. The decision on which ensemble gives the right answer depends, of course, on the particular situation; if it were feasible to come up with an experiment that conforms to the grand canonical ensemble, the large grand canonical fluctuations should actually be observed. At present, experiments with dilute Bosonic atoms in magnetic, magneto-optical or optical traps [4] fall into the realms of the microcanonical ensemble, once the evaporative cooling process has come to an end and the state of equilibrium is reached. In contrast, the experiments of Reppy and co-workers [5] performed with ^{4}He in a porous medium are much closer to the physics of the canonical ensemble: In this case the contact with the host medium (vycor glass) entails heat exchange, while the particle number is held constant.

Within the canonical ensemble studied in this paper, a partially condensed ideal Bose gas is equivalent to a system of uncoupled harmonic oscillators. This is expressed most clearly by the partition function (38); the only approximation required to establish this (almost-) equivalence is stated in Eq. (37). Pictorially speaking, adopting this approximation means replacing the finite condensate by an infinite reservoir of condensate particles, as suggested by Fierz already in 1956 [22], and, more recently, by Navez et al. in the context of the "Maxwell's demon ensemble" [21]. This allows one to bypass the canonical constraint of fixed particle number N, and to treat canonical statistics in great analytical detail. The central result of this work, the cumulant formula (39) and its integral representation (56), furnishes a direct link between single-particle spectrum and condensate statistics.

The integral representation (56) of the cumulant formula is distinguished by its conceptual clarity. For a specific trap, the kth cumulant is determined by the pole structure of the product $Z(\beta,t)\,\zeta(t+1-k)$ in the complex t-plane, the first factor incorporating the trap properties, the second the cumulant order. The large-system behavior is extracted from the leading pole, finite-size corrections are encoded in the next-to-leading poles, and the non-Gaussian nature of the condensate fluctuations is immediately visible. We have taken some effort to show in detail how the generalized Zeta functions $Z(\beta,t)$ appear in a natural manner, and have considered three particular examples. Actually, such Zeta functions play a prominent role in several areas of mathematical physics, and there exists a substantial amount of knowledge about them [39], so that the investigation of other traps, with other single-particle spectra, poses no problem.

The master equation approach to canonical condensate statistics [6,7] has other, distinct merits. It is not limited to the condensate regime and in principle reproduces the canonical ensemble statistics exactly [10]; approximations enter only when the exact values of the heating and cooling coefficients (2) and (3) are not known. Within the mean field-like quasithermal approximation (5) introduced for calculating these coefficients, it describes the statistics of the ground state occupation number quite well even in the transition regime to the condensate. One might perhaps feel tempted to improve this quasithermal approximation, and to introduce further parameters besides the two basic parameters $\mathscr{H}$ and η, such that, for instance, also skewness and flatness of the distributions (28) are reproduced perfectly. This can be done, but it might well be counterproductive. The actual virtue of the master equation lies in the fact that it appeals to the intuition, and yields reliable results even within the scope of simple, physically well motivated approximations. Therefore, one may hope to develop a similar approach for studying, with equal transparency, condensate statistics in interacting Bose gases.

One might wonder why one should pay so much attention to the ideal Bose gas, arguing that an interacting gas might behave in an entirely different manner. The well-studied example of a weakly interacting, homogeneous Bose gas in a box with periodic boundary conditions suggests that, on the contrary, many of the structures encountered in this paper are preserved when the interaction is turned on. In particular, while the ideal gas corresponds to a system of uncoupled harmonic oscillators, the Bogoliubov approximation leads to pairwise coupling between such oscillators—an oscillator corresponding to a particle with momentum $\mathbf{k}$ is coupled only to its counterpart with momentum $-\mathbf{k}$—, so that at low temperatures the number of degrees of freedom in the interacting gas is effectively half the number one finds in the ideal case [17,18]. As a consequence, in comparison with the ideal gas all cumulants for the interacting system are merely suppressed by a factor of 2. This relation between the interacting and the ideal gas, first observed for the fluctuation Δn_0^2 of a weakly interacting, homogeneous condensate by Giorgini et al. [40] and extended to arbitrary interaction strength in Ref. [41], is thus far from being accidental. In view of the examples studied in Section 5, it would be instructive to evaluate the condensate statistics for the weakly interacting Bose gas in a box with hard walls, and for other types of traps. After all, a "periodic" box and a hard-walled one are two different systems, with *quite* different single-particle ground states, so that some differences between the respective fluctuation characteristics should remain at least for weak interactions. It would be interesting to explore if, and to what extent, the increase of the interaction strength wipes out the difference between the fluctuation properties of mesoscopic condensates in different traps.

Acknowledgements

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Appendix A. Poles and residues of generalized Zeta functions

In this appendix, we explain briefly how to compute the locations of the poles of analytically continued generalized Zeta functions (52), and their residues. We focus on the homogeneous and inhomogeneous Epstein Zeta functions encountered in Eqs. (76) and (89), but the same scheme can be employed in general. For further details and references, we point to the exhaustive articles by Kirsten [34,42]. The key point consists in the following observation [39]:

If $0 < \lambda_1 \leqslant \lambda_2 \leqslant \lambda_3 \leqslant \cdots$ is a sequence of real numbers with $\lambda_\nu \to \infty$, such that the partition function

$$\Theta(\beta) = \sum_{\nu=1}^{\infty} \exp(-\beta\lambda_\nu) \tag{A.1}$$

converges for $\mathrm{Re}(\beta) > 0$, and possesses for $\beta \to 0$ (i.e., for high temperatures) the asymptotic expansion

$$\Theta(\beta) \sim \sum_{n=0}^{\infty} c_{i_n} \beta^{i_n} \tag{A.2}$$

with a strictly increasing sequence of real exponents i_n starting with a negative number $i_0 < 0$, then $\Theta(\beta)$ admits, for $\mathrm{Re}(t) > -i_0$, a Mellin transform $\mathscr{M}\Theta(t)$, defined by

$$\mathscr{M}\Theta(t) = \int_0^\infty \mathrm{d}\beta\, \beta^{t-1}\Theta(\beta)\,; \tag{A.3}$$

this Mellin transform exhibits simple poles at $t = -i_n$ with residues c_{i_n}. The associated Zeta function, that is, the analytic continuation of

$$Z(t) = \sum_{v=1}^{\infty} \frac{1}{\lambda_v^t}\,, \tag{A.4}$$

is then given by

$$Z(t) = \frac{1}{\Gamma(t)} \mathscr{M}\Theta(t)\,. \tag{A.5}$$

Therefore, there are potential poles of $Z(t)$ at

$$t = -i_n \quad \text{with residue } c_{i_n}/\Gamma(-i_n)\,; \tag{A.6}$$

keeping in mind that the singularities of the Gamma function will eliminate those poles of $\mathscr{M}\Theta(t)$ that are located at zero or negative integer numbers. This connection provides the strategy we have to follow: Given some Zeta function of the form (A.4), defined for such t which render the sum absolutely convergent, we focus on the corresponding partition function (A.1) and find its asymptotic (high-temperature) expansion (A.2). The exponents and coefficients emerging in this expansion then provide, by means of Eq. (A.6), the positions and residues of the poles of the analytically continued Zeta function.

To see how this works in practice, let us first study the Zeta function

$$E_1(t) = \sum_{n=1}^{\infty} (n^2)^{-t}\,. \tag{A.7}$$

To find expansion (A.2), we recall the Poisson resummation formula

$$\sum_{n=-\infty}^{+\infty} \exp(-\beta n^2) = \left(\frac{\pi}{\beta}\right)^{1/2} \sum_{n=-\infty}^{+\infty} \exp(-\pi^2 n^2/\beta)\,, \tag{A.8}$$

and rearrange it to read

$$\sum_{n=1}^{\infty} \exp(-\beta n^2) = \frac{1}{2}\left[\left(\frac{\pi}{\beta}\right)^{1/2} - 1 + 2\left(\frac{\pi}{\beta}\right)^{1/2} \sum_{n=1}^{\infty} \exp(-\pi^2 n^2/\beta)\right]. \tag{A.9}$$

Seen from the viewpoint of statistical mechanics, this identity links the low-temperature behavior ($\beta \to \infty$ on the left-hand side) of the partition function of a system with quadratic spectrum to its high-temperature counterpart ($1/\beta \to \infty$ on the right-hand side). Leaving out those terms in Eq. (A.9) that are exponentially damped for $\beta \to 0$, we arrive at the required asymptotic expansion,

$$\sum_{n=1}^{\infty} \exp(-\beta n^2) \sim \frac{1}{2}\left(\frac{\pi}{\beta}\right)^{1/2} - \frac{1}{2}\,. \tag{A.10}$$

Thus, we have $i_0 = -\frac{1}{2}$, $c_{i_0} = \sqrt{\pi}/2$, and $i_1 = 0$, $c_{i_1} = -\frac{1}{2}$; all other coefficients c_{i_n} vanish. Since the Gamma function is singular at $t = 0$, the analytic continuation of $E_1(t)$ has merely a single pole, located at

$$t = -i_0 = 1/2 \quad \text{with residue } \frac{c_{-1/2}}{\Gamma(1/2)} = \frac{1}{2} \,. \tag{A.11}$$

Of course, since $E_1(t) = \zeta(2t)$, we could also have inferred this result from Eq. (60). But now we got our machinery running: Multiplying the expansion (A.10) with itself, we find

$$\sum_{n_1,n_2=1}^{\infty} \exp(-\beta(n_1^2 + n_2^2)) \sim \frac{\pi}{4\beta} - \frac{1}{2}\left(\frac{\pi}{\beta}\right)^{1/2} + \frac{1}{4} \,, \tag{A.12}$$

implying that the Epstein function $E_2(t)$ defined in Eq. (76) has poles at

$$t = 1, 1/2 \quad \text{with residues } \frac{\pi}{4}, -\frac{1}{2} \,. \tag{A.13}$$

Multiplying then Eq. (A.10) by Eq. (A.12), we arrive at

$$\sum_{n_1,n_2,n_3=1}^{\infty} \exp(-\beta(n_1^2 + n_2^2 + n_3^2)) \sim \frac{1}{8}\left(\frac{\pi}{\beta}\right)^{3/2} - \frac{3\pi}{8\beta} + \frac{3}{8}\left(\frac{\pi}{\beta}\right)^{1/2} - \frac{1}{8} \,, \tag{A.14}$$

stating that $E_3(t)$ has poles at

$$t = 3/2, 1, 1/2 \quad \text{with residues } \frac{\pi}{4}, -\frac{3\pi}{8}, \frac{3}{8} \,. \tag{A.15}$$

Next, we turn to the inhomogeneous Epstein functions introduced in Eq. (89). The partition function associated with $\tilde{E}_1(t)$, namely

$$\Theta(\beta) = \exp(\beta) \sum_{n=2}^{\infty} \exp(-\beta n^2) \,, \tag{A.16}$$

forces us to rewrite identity (A.8) as

$$\sum_{n=2}^{\infty} \exp(-\beta n^2) = \frac{1}{2}\left[\left(\frac{\pi}{\beta}\right)^{1/2} - 1 - 2\exp(-\beta) + 2\left(\frac{\pi}{\beta}\right)^{1/2} \sum_{n=1}^{\infty} \exp(-\pi^2 n^2/\beta)\right] \,. \tag{A.17}$$

Again discarding terms that are exponentially damped for $\beta \to 0$, multiplying by $\exp(\beta)$, and expanding this latter exponential, we find

$$\sum_{n=2}^{\infty} \exp(-\beta(n^2 - 1)) \sim \frac{1}{2}\left(\frac{\pi}{\beta}\right)^{1/2} - \frac{3}{2} + \frac{(\pi\beta)^{1/2}}{2} - \frac{\beta}{2} + \cdots \,. \tag{A.18}$$

In contrast to its counterpart (A.10), this expansion in powers of $\beta^{1/2}$ does not terminate, so that $\tilde{E}_1(t)$ possesses infinitely many poles. For our purposes, it will be sufficient to account for only the leading of these poles, located at

$$t = \tfrac{1}{2} \quad \text{with residue } \tfrac{1}{2} \,. \tag{A.19}$$

Multiplying Eq. (A.18) by itself, we obtain

$$\sum_{n_1,n_2=2}^{\infty} \exp(-\beta(n_1^2+n_2^2-2)) \sim \frac{\pi}{4\beta} - \frac{3}{2}\left(\frac{\pi}{\beta}\right)^{1/2} + \frac{2\pi+9}{4} - 2(\pi\beta)^{1/2} + \cdots , \tag{A.20}$$

so that the leading poles of $\tilde{E}_2(t)$ are found at

$$t = 1, 1/2 \quad \text{with residues } \frac{\pi}{4}, -\frac{3}{2} . \tag{A.21}$$

Finally, multiplying Eq. (A.18) by Eq. (A.20) results in

$$\sum_{n_1,n_2,n_3=2}^{\infty} \exp(-\beta(n_1^2+n_2^2+n_3^2-3)) \sim \frac{1}{8}\left(\frac{\pi}{\beta}\right)^{3/2} - \frac{9\pi}{8\beta} + \frac{27+3\pi}{8}\left(\frac{\pi}{\beta}\right)^{1/2} + \cdots , \tag{A.22}$$

from which we deduce in the usual manner that the leading poles of $\tilde{E}_3(t)$ lie at

$$t = 3/2, 1, 1/2 \quad \text{with residues } \frac{\pi}{4}, -\frac{9\pi}{8}, \frac{27+3\pi}{8} . \tag{A.23}$$

Comparing the poles and residues of the inhomogeneous Zeta functions $\tilde{E}_d(t)$ to those of their homogeneous counterparts $E_d(t)$, we see that neither the positions nor the residues of the leading poles at $t = d/2$ are affected by the inhomogeneity, whereas the next-to-leading poles of $\tilde{E}_d(t)$, which are found at the same positions as those of $E_d(t)$ for $d \geqslant 2$, already exhibit a different residue.

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