

Condensation of ideal Bose gas confined in a box within a canonical ensemble

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We set up recursion relations for the partition function and the ground-state occupancy for a fixed number of noninteracting bosons confined in a square box potential and determine the temperature dependence of the specific heat and the particle number in the ground state. A proper semiclassical treatment is set up which yields the correct small- T behavior in contrast to an earlier theory in Feynman's textbook on statistical mechanics, in which the special role of the ground state was ignored. The results are compared with an exact quantum-mechanical treatment. Furthermore, we derive the finite-size effect of the system.

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I. INTRODUCTION

The thermodynamic properties of a Bose gas are usually studied in the grand-canonical formulation where energy and particle number are fixed on the average. Present day experiments, on the other hand, are performed in a magnetic or optical trap which contain a roughly fixed number of particles. Thus, the experimental situation may be better approximated by a canonical ensemble with fixed particle number. In the thermodynamic limit one usually expects grand-canonical and canonical treatments to yield the same results for all thermodynamic quantities and the condensate fraction. This has indeed been proved in [1] in general and for harmonic traps in [2–5]. Some statistical quantities, however, do not have the same thermodynamic limits in the two ensembles. One fundamental example is the fluctuation width $\Delta N_0 \equiv \sqrt{\langle (\Delta N_0)^2 \rangle}$ of the particle number N_0 in the ground state. In the grand-canonical ensemble, this quantity has the size $\sqrt{N_0(N_0+1)}$ and is at low temperatures T of the order of the total particle number N [1,2,6–8]. In the canonical ensemble, on the other hand, this quantity can be shown to vanish at $T=0$ since N_0 becomes equal to the fixed particle number N . The grand-canonical result is a consequence of the assumed statistical independence of all open grand-canonical subsystems. This assumption is only fulfilled if there is no long-range ordered condensate, otherwise it is wrong. The problem can be properly removed by fixing the whole particle number and ignoring its fluctuations as was shown, e.g., in [1,6]. The particle number in the ground state is then $N_0=N-N_{\text{ex}}$, where N_{ex} is the excited particle number. Since, furthermore, the fluctuation ΔN_{ex} of the thermal gas, consisting of excited states, can be shown to vanish for zero temperature, the same is true for ΔN_0 . Its temperature behavior is found to be $\Delta N_0 \sim (T/T_c)^{3/2}N^{1/2}$ for an ideal gas in a harmonic trap [2] and $\Delta N_0 \sim (T/T_c)N^{2/3}$ for a homogeneous system [9] for temperatures T below its critical value T_c . By

fixing the full particle number N , the system does not exchange its particles with the environment at all and this situation, therefore, corresponds to one in a canonical ensemble. The only exception is that excited states are then still described by the grand-canonical Bose-Einstein distribution. The entire canonical description will be presented below.

The canonical treatment is conveniently performed in a first-quantized path-integral description. All particles are represented by cycles winding around a cylinder in Euclidean space time whose circumference is the imaginary-time axis $\tau \in (0, \hbar/k_B T)$ [10,11]. For sufficiently low temperatures, the indistinguishability of particles leads to long closed paths winding many times around this cylinder, giving rise to correlated subsets of particles [12]. In Ref. [13], this representation was utilized to claim that condensation amounts directly to a proliferation of long cycles. This claim can, however, not be upheld. The formation of correlated collectives is the origin of superfluidity, not condensation, as it was correctly implemented for an ideal gas in a harmonic trap [14]. The essential signal for the Bose-Einstein condensation is, instead, associated with the occupancy of the single-particle ground state. Thus, not the winding numbers of the cycles are relevant to condensation, but the weight of the ground state in them. For a harmonic trap, this was properly shown in Refs. [15,16].

If the harmonic trap is replaced by a square box, whose infinite-volume limit is the homogeneous system, the systems confined in it show some unusual features. It is the purpose of this paper to exhibit these. The discussion starts in Sec. II with a brief summary of the imaginary-time evolution amplitude for a fixed number N of bosons, where the indistinguishability of particles is explicitly taken into account. In Sec. III we calculate the partition function of such a canonical system from the trace of the N -particle imaginary-time evolution amplitude written in the cycle representation of paths. Since this is hard to evaluate numerically for a large particle number, we have derived an efficient recursion relation along the lines of Refs. [5,17–20] in Sec. IV. In Sec. V this relation is made specific by a spectral decomposition of the canonical partition function. This allows us in Sec. VI to extract the ground-state contribution to

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the partition function from the cycle representation, from which we read off the probability to find a particle in the ground state. This is used to define the condensate fraction N_0/N for a system with a fixed particle number N . In Sec. VII we apply our results to the Bose gas confined in the square box potential. There we show that the semiclassical approximation requires a delicate treatment of the ground state for finite systems. This is necessary in order to obtain the correct low-temperature behavior of the thermodynamical functions in contrast to an earlier theory in Feynman's original textbook [10]. The results are then compared with an exact quantum-mechanical calculation. In Sec. VIII we investigate the finite-size effect in a box potential. We identify a would-be transition temperature as the finite- N version of the critical temperature of Bose-Einstein condensation in a canonical ensemble. Subsequently, canonical results calculated for these crossover temperatures are compared with grand-canonical ones. We end with an analytic calculation of the finite-size effect upon the critical temperature in the grand-canonical ensemble.

II. QUANTUM STATISTICS OF IDENTICAL PARTICLES

We start by briefly reviewing the quantum statistics of a fixed number N of noninteracting identical particles in a first quantized approach [10,11]. At first, they are treated as distinguishable particles. Their orbits in imaginary time τ are denoted by $\mathbf{x}_\nu(\tau)$ with the particle indices $\nu=1,2,\dots,N$. Global and local thermodynamic properties of the many-particle system are determined by the imaginary-time evolution amplitude which is given by the path integral

$$\begin{aligned} & (\mathbf{x}_{1b}, \dots, \mathbf{x}_{Nb}, \tau_b | \mathbf{x}_{1a}, \dots, \mathbf{x}_{Na}, \tau_a) \\ &= \left(\prod_{\nu=1}^N \int_{\mathbf{x}_\nu(\tau_a)=\mathbf{x}_{\nu a}}^{\mathbf{x}_\nu(\tau_b)=\mathbf{x}_{\nu b}} \mathcal{D}\mathbf{x}_\nu \right) e^{-\mathcal{A}[\mathbf{x}_1, \dots, \mathbf{x}_N]/\hbar}. \end{aligned} \quad (1)$$

The Euclidean action in the exponent has the generic form

$$\mathcal{A}[\mathbf{x}_1, \dots, \mathbf{x}_N] = \sum_{\nu=1}^N \int_{\tau_a}^{\tau_b} d\tau \left(\frac{M}{2} \dot{\mathbf{x}}_\nu^2(\tau) + V[\mathbf{x}_\nu(\tau)] \right) \quad (2)$$

with the particle mass M and the common background potential $V(\mathbf{x}_\nu)$ for all particles. Due to the additive of the action (2) we find that the imaginary-time evolution amplitude of N distinguishable noninteracting particles factorizes into N one-particle amplitudes

$$\begin{aligned} & (\mathbf{x}_{1b}, \dots, \mathbf{x}_{Nb}, \tau_b | \mathbf{x}_{1a}, \dots, \mathbf{x}_{Na}, \tau_a) \\ &= (\mathbf{x}_{1b}, \tau_b | \mathbf{x}_{1a}, \tau_a) \cdots (\mathbf{x}_{Nb}, \tau_b | \mathbf{x}_{Na}, \tau_a). \end{aligned} \quad (3)$$

These one-particle amplitudes fulfill the semigroup property

$$(\mathbf{x}_c, \tau_c | \mathbf{x}_a, \tau_a) = \int d^3x_b (\mathbf{x}_c, \tau_c | \mathbf{x}_b, \tau_b) (\mathbf{x}_b, \tau_b | \mathbf{x}_a, \tau_a) \quad (4)$$

and are invariant with respect to translations in the imaginary time

$$(\mathbf{x}_b, \tau_b + \tau_0 | \mathbf{x}_a, \tau_a + \tau_0) = (\mathbf{x}_b, \tau_b | \mathbf{x}_a, \tau_a). \quad (5)$$

We now impose the indistinguishability of particles. In $D > 2$ space dimensions there are only two kinds of indistin-

guishable particles: bosons with a completely symmetric and fermions with a completely antisymmetric N -particle wave function. According to Pauli's spin-statistic theorem they are associated with integer and half-integer spins, respectively. The corresponding modifications of the path integral (1) are straightforward. For bosons, we must sum over all permuted final positions $\mathbf{x}_{P(\nu)b}$, where $P(\nu)$ denotes one of the $N!$ possible permutations of the index ν . For fermions, there is an extra minus sign for odd permutations. Restricting ourselves in this paper to the bosonic case, we must calculate the imaginary-time evolution amplitude

$$\begin{aligned} & (\mathbf{x}_{1b}, \dots, \mathbf{x}_{Nb}, \tau_b | \mathbf{x}_{1a}, \dots, \mathbf{x}_{Na}, \tau_a)^B \\ &= \frac{1}{N!} \sum_P (\mathbf{x}_{P(1)b}, \dots, \mathbf{x}_{P(N)b}, \tau_b | \mathbf{x}_{1a}, \dots, \mathbf{x}_{Na}, \tau_a). \end{aligned} \quad (6)$$

III. CYCLE EXPANSION

The canonical partition function of N noninteracting bosons is given by the trace

$$Z_N^B(\beta) = \int d^3x_1 \cdots \int d^3x_N \langle \mathbf{x}_1, \dots, \mathbf{x}_N, \hbar\beta | \mathbf{x}_1, \dots, \mathbf{x}_N, 0 \rangle^B, \quad (7)$$

where $\beta \equiv (k_B T)^{-1}$ represents the reciprocal temperature. The calculation of this basic statistic quantity is nontrivial due to the indistinguishability of the particles. At first we consider the Bose gas with small particle numbers N . For $N=1$, the partition function (7) reduces to the well-known expression

$$Z_1(\beta) = \int d^3x \langle \mathbf{x}, \hbar\beta | \mathbf{x}, 0 \rangle. \quad (8)$$

Here we have omitted the index B , as the distinguishable particles are not an issue for a single particle. For $N=2$, we obtain from (7) according to the indistinguishability of (6) and the factorization property (3)

$$\begin{aligned} Z_2^B(\beta) &= \frac{1}{2!} \int d^3x_1 d^3x_2 [(\mathbf{x}_1, \hbar\beta | \mathbf{x}_1, 0)(\mathbf{x}_2, \hbar\beta | \mathbf{x}_2, 0) \\ &+ (\mathbf{x}_2, \hbar\beta | \mathbf{x}_1, 0)(\mathbf{x}_1, \hbar\beta | \mathbf{x}_2, 0)]. \end{aligned} \quad (9)$$

Using the translational invariance (5) together with the semigroup property (4) for the second term, this yields with (8),

$$Z_2^B(\beta) = \frac{1}{2} [Z_1^2(\beta) + Z_1(2\beta)]. \quad (10)$$

In a similar way, we obtain the result for $N=3$,

$$Z_3^B(\beta) = \frac{1}{6} [Z_1^3(\beta) + 3Z_1(\beta)Z_1(2\beta) + 2Z_1(3\beta)]. \quad (11)$$

For an arbitrary number N of bosons we must calculate according to (3) and (6) the canonical partition function (7),

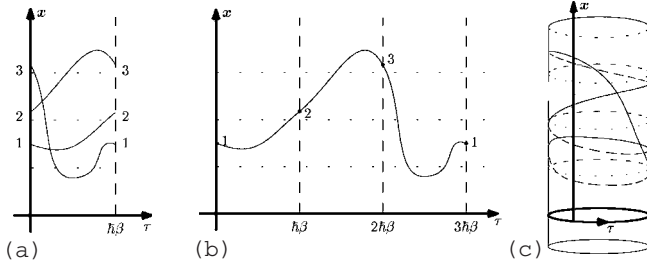


FIG. 1. Example of paths contributing to (13) for a cycle of length $n=3$: (a) final points coincide with initial points of the other particles, (b) and (c) show the same situation in an extended zone scheme and wrapped upon a cylinder, respectively. See Ref. [13].

$$Z_N^B(\beta) = \frac{1}{N!} \sum_P \int d^3x_1 \cdots \int d^3x_N (\mathbf{x}_{P(1)}, \hbar\beta | \mathbf{x}_1, 0) \cdots (\mathbf{x}_{P(N)}, \hbar\beta | \mathbf{x}_N, 0). \quad (12)$$

Due to the indistinguishability of the particles there are single-particle amplitudes contributing to the partition function (12), whose final points coincide with the initial points of other particles. These amplitudes can be combined to many-particle formations, which can be represented by paths winding around a cylinder of circumference $\hbar\beta$. A typical situation for three particles is shown in Fig. 1. This represents a single closed cycle with three windings around the cylinder. An arbitrary single cycle with n windings is given by the multiple integral

$$Z_n^c(\beta) = \int d^3x_1 \cdots \int d^3x_n (\mathbf{x}_1, \hbar\beta | \mathbf{x}_n, 0) \times (\mathbf{x}_n, \hbar\beta | \mathbf{x}_{n-1}, 0) \cdots (\mathbf{x}_3, \hbar\beta | \mathbf{x}_2, 0) (\mathbf{x}_2, \hbar\beta | \mathbf{x}_1, 0). \quad (13)$$

Due to the translational invariance (5) and the semigroup property (4) of the one-particle imaginary-time evolution amplitude we see that

$$Z_n^c(\beta) = Z_1(n\beta). \quad (14)$$

Thus, a contribution of a closed cycle of length n corresponds to a simple one-particle partition function but with a temperature scaled down by the same factor n . With this we return to the general expression (12) for the canonical partition function. The full N -particle partition function decomposes into mutually disconnected groups of closed paths winding around a cylinder of circumference $\hbar\beta$. Due to the indistinguishability of particles this decomposition is non-trivial since the cycles may have different winding numbers.

In order to illustrate the situation, we consider in detail the possible path combinations for $N=2$ and $N=3$ particles. Figure 2 shows the respective permutations in different notations. In the cycle notation the indices of particles contributing to the closed paths are stated within parentheses. This cycle notation is mathematically useful but is not adopted to the indistinguishability of particles as it relies explicitly on the numbering of the particles. For instance, the second, third, and fourth permutation in the second row of Fig. 2 are

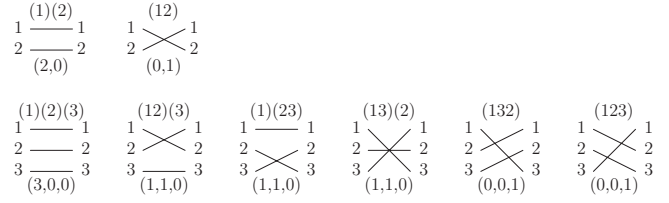


FIG. 2. Permutations for $N=2$ (first row) and $N=3$ (second row) particles. The indices above each permutation stand for the cycle notation, whereas the respective N -tuple (C_1, \dots, C_N) below each permutation denotes the cycle number notation.

regarded as different permutations, although they are identical from the physical point of view. This motivates us to introduce a different notation for the permutations which respects the indistinguishability of the particles. It is the cycle-number notation which characterizes each permutation by the N -tuple (C_1, \dots, C_N) of numbers C_n of cycles with the length n . In this notation the second, third, and fourth permutations in the second row of Fig. 2 have the same 3-tuple $(1,1,0)$.

Using the result (14) for the multiple integral (13) we arrive at the cycle decomposition of the canonical partition function (12),

$$Z_N^B(\beta) = \frac{1}{N!} \sum_P \prod_{n=1}^{\sum_n C_n n = N} [Z_1(n\beta)]^{C_n}. \quad (15)$$

Note that the numbers of cycles C_n of length n , which occur for a certain permutation P , are restricted by the condition $\sum_n C_n n = N$. The sum in (15) can be rearranged as follows. Instead of summing over permutations and decomposing them into cycles, we may sum directly over all different cycle numbers (C_1, \dots, C_N) which respect the equation $\sum_n C_n n = N$. By doing so, we must take into account that a particular configuration (C_1, \dots, C_N) can occur with a certain multiplicity $M(C_1, \dots, C_N)$. For instance, in Fig. 2 we can read off $M(3,0,0)=1$, $M(1,1,0)=3$, and $M(0,0,1)=2$ for three particles. Thus, we obtain

$$Z_N^B(\beta) = \frac{1}{N!} \sum_{C_1, \dots, C_N}^{\sum_n C_n n = N} M(C_1, \dots, C_N) \prod_{n=1}^{\infty} [Z_1(n\beta)]^{C_n}, \quad (16)$$

where we have formally extended the product to all integers by setting $C_n=0$ for any $n > N$ due to the condition $\sum_n C_n n = N$.

Now we derive a general formula for the multiplicities $M(C_1, \dots, C_N)$. In total the cycle numbers (C_1, \dots, C_N) can be arranged in $N!$ different combinations. However, not all of those represent different permutations as we shall demonstrate by the following examples.

(i) The cycle numbers $(C_1=0, C_2=0, C_3=1)$ allow for six combinations $(123), (312), (231), (132), (213), (321)$, where the former and latter three combinations are different representations of only two permutations,

$$P_1 = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix}, \quad P_2 = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}. \quad (17)$$

(ii) The cycle numbers ($C_1=3, C_2=0, C_3=0$) lead to six combinations (1)(2)(3), (1)(3)(2), (2)(1)(3), (2)(3)(1), (3)(1)(2), (3)(2)(1) which are all representations of the same permutation

$$P_3 = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \end{pmatrix}. \quad (18)$$

These observations are generalized as follows:

(i) A cyclic permutation within a n cycle does not lead to a new permutation, so we have n irrelevant combinations.

(ii) Exchanging cycles of the same length does not lead to a new permutation, so we have $C_n!$ irrelevant combinations.

Summarizing these combinatorial considerations, we obtain for the multiplicity the Cauchy formula of the permutation group [21,22],

$$M(C_1, \dots, C_N) = \frac{N!}{\prod_n C_n! n^{C_n}}. \quad (19)$$

After this combinatorial excursion we return to the canonical partition function (16). Using (19), we find our second main result in the form of a cycle representation of the canonical partition function [10],

$$Z_N^B(\beta) = \sum_{C_1, \dots, C_N} \prod_{n=1}^{\infty} \frac{1}{C_n!} \left(\frac{Z_1(n\beta)z^n}{n} \right)^{C_n}. \quad (20)$$

Note that specializing (20) for $N=2$ and $N=3$ particles reproduces, indeed, the earlier findings (10) and (11).

Although the cycle representation allows us, in principle, to determine the canonical partition function $Z_N^B(\beta)$, this approach is not efficient for a large particle number N as the computational effort grows as a factorial with N . Furthermore, it is rather cumbersome to figure out all cycle numbers C_n which respect the condition $\sum_n C_n n = N$. Therefore, we need to find a more efficient algorithm to determine canonical partition functions. This is done by using the fact that the grand-canonical partition function is the generating function of all canonical partition functions [19].

IV. GENERATING FUNCTION AND RECURSION RELATION

Introducing the fugacity $z \equiv e^{\beta\mu}$ with the chemical potential μ , the grand-canonical partition function reads

$$\mathcal{Z}_{GC}^B(\beta, z) = \sum_{N=0}^{\infty} Z_N^B(\beta) z^N. \quad (21)$$

This quantity serves as the generating function of canonical partition functions $Z_N^B(\beta)$, which are simply the Taylor expansion coefficients

$$Z_N^B(\beta) = \frac{1}{N!} \left. \frac{\partial^N \mathcal{Z}_{GC}^B(\beta, z)}{\partial z^N} \right|_{z=0}. \quad (22)$$

In order to evaluate (21), we use the cycle representation (20) and insert the condition $N = \sum_n C_n n$ into the exponent of the fugacity z . Thus, we obtain at first

$$\begin{aligned} \mathcal{Z}_{GC}^B(\beta, z) &= \sum_{N=0}^{\infty} \sum_{C_1, \dots, C_N} \prod_{n=1}^{\infty} \frac{1}{C_n!} \left(\frac{Z_1(n\beta)z^n}{n} \right)^{C_n} \\ &= \sum_{C_1=0}^{\infty} \sum_{C_2=0}^{\infty} \dots \prod_{n=1}^{\infty} \frac{1}{C_n!} \left(\frac{Z_1(n\beta)z^n}{n} \right)^{C_n}. \end{aligned} \quad (23)$$

In the second expression the condition $\sum_n C_n = N$ no longer occurs. Due to this simplification we can rewrite the multiple sum over the cycle numbers C_n as a product over the individual sums and obtain

$$\mathcal{Z}_{GC}^B(\beta, z) = \prod_{n=1}^{\infty} \sum_{C_n=0}^{\infty} \frac{1}{C_n!} \left(\frac{Z_1(n\beta)z^n}{n} \right)^{C_n}. \quad (24)$$

Performing the C_n summation yields the result

$$\mathcal{Z}_{GC}^B(\beta, z) = \exp \left(\sum_{n=1}^{\infty} \frac{Z_1(n\beta)z^n}{n} \right). \quad (25)$$

The partition function of the vacuum, where no particle is present ($N=0$), is obviously found from (22) with (25),

$$Z_0^B(\beta) = 1. \quad (26)$$

For $N \geq 1$, we observe that the grand-canonical partition function (25) obeys the differential equation

$$\frac{\partial \mathcal{Z}_{GC}^B(\beta, z)}{\partial z} = \mathcal{Z}_{GC}^B(\beta, z) \sum_{k=1}^{\infty} Z_1(k\beta) z^{k-1}. \quad (27)$$

This is a self-consistent equation for the generating function which we solve recursively. Forming the N th derivative of (21) via the Leibniz rule of differentiation,

$$\begin{aligned} \left. \frac{\partial^N \mathcal{Z}_{GC}^B(\beta, z)}{\partial z^N} \right|_{z=0} &= \sum_{n=1}^N \frac{(N-1)!}{(n-1)!(N-n)!} \left. \frac{\partial^{N-n} \mathcal{Z}_{GC}^B(\beta, z)}{\partial z^{N-n}} \right|_{z=0} \\ &\quad \times \sum_{k=1}^{\infty} Z_1(k\beta) \left. \frac{\partial^{n-1} z^{k-1}}{\partial z^{n-1}} \right|_{z=0}, \end{aligned} \quad (28)$$

and taking into account the identity

$$\left. \frac{\partial^{n-1} z^{k-1}}{\partial z^{n-1}} \right|_{z=0} = (n-1)! \delta_{k,n}, \quad (29)$$

we obtain from (22) the desired recursion relation for the canonical partition functions $Z_N^B(\beta)$ [5,17–20],

$$Z_N^B(\beta) = \frac{1}{N} \sum_{n=1}^N Z_1(n\beta) Z_{N-n}^B(\beta). \quad (30)$$

Inserting the starting value (26), we immediately reproduce for $N=2$ and $N=3$ the earlier results (10) and (11). For large particle numbers it can be shown that the computational effort grows only algebraically with N . Thus, iterating Eq. (30) can be done very efficiently, as is further worked out in Ref. [18].

Once we have obtained the N -particle partition function, we can proceed to calculate all thermodynamic quantities of interest. For instance, in Sec. VII we shall determine the specific heat capacity according to

$$C_N^B(T) = k_B T \frac{\partial^2}{\partial T^2} (T \ln Z_N^B). \quad (31)$$

V. SPECTRAL DECOMPOSITION

In order to apply the recursion relation (30) to specific systems we must calculate the one-particle partition function $Z_1(\beta)$ of Eq. (8). For this we solve the time-independent Schrödinger equation and use the energy eigenvalues $E_{\mathbf{k}}$ to calculate $Z_1(\beta)$ as a spectral sum

$$Z_1(\beta) = \sum_{\mathbf{k}} e^{-\beta E_{\mathbf{k}}}, \quad (32)$$

where \mathbf{k} stands for the quantum numbers. The n -fold cycle (14),

$$Z_n^c(\beta) = \sum_{\mathbf{k}} e^{-\beta(nE_{\mathbf{k}})} \quad (33)$$

may be interpreted physically as a partition function (32) of a single quasiparticle consisting of a correlated union of n fundamental particles with the total energy $nE_{\mathbf{k}}$.

The spectral representation (32) leads via (25) to the grand-canonical partition function

$$Z_{GC}^B(\beta, \mu) = \exp\left(-\sum_{\mathbf{k}} \ln(1 - e^{-\beta(E_{\mathbf{k}} - \mu)})\right). \quad (34)$$

From it we may derive the average particle number in a grand-canonical ensemble according to

$$\langle N \rangle = \frac{1}{\beta} \frac{\partial}{\partial \mu} [\ln Z_{GC}^B(\beta, \mu)] = \sum_{\mathbf{k}} \frac{1}{e^{\beta(E_{\mathbf{k}} - \mu)} - 1}, \quad (35)$$

which is the well-known Bose-Einstein distribution.

VI. GROUND-STATE OCCUPANCY

The most important physical quantity in Bose-Einstein condensation is the condensate fraction N_0 which is also called the ground-state occupancy. In the usual grand-canonical treatment this quantity is found by solving numerically the Bose-Einstein distribution (35) [19,20]. To this end one calculates the chemical potential μ for a given temperature T at a fixed average particle number $\langle N \rangle$. Given $\mu(T)$ one finds the average number of particles in the ground-state fraction from the equation $\langle N_0 \rangle = (e^{\beta(E_G - \mu)} - 1)^{-1}$, where E_G is the ground-state energy.

In the present paper we shall treat this problem canonically at a fixed particle number N , without fixing a chemical potential. To this end we calculate directly the probability that one of the bosons resides in its ground state [15,16]. This probability multiplied by N will be considered to be the finite- N version of the condensate fraction N_0 . In order to determine this quantity, we isolate in Sec. VI A the ground-state contribution to the cycle representation (20). Subsequently, in Sec. VI B, we derive a more efficient equation for the canonical ground-state occupancy.

A. Cycle representation

Using the spectral decomposition (32), we can rewrite $Z_1(n\beta)$ according to

$$Z_1(n\beta) = \gamma_n(\beta) + \xi_n(\beta). \quad (36)$$

The first term denotes the contribution of the ground state

$$\gamma_n(\beta) = e^{-n\beta E_G}, \quad (37)$$

where E_G denotes the ground-state energy. The second term in (36) stems from all excited states

$$\xi_n(\beta) = \sum'_{\mathbf{n}} e^{-n\beta E_{\mathbf{n}}}, \quad (38)$$

where the prime indicates the omission of the ground state. Using the binomial formula, the canonical partition function (20) is then decomposed as follows:

$$Z_N^B(\beta) = \sum_{C_1, \dots, C_N}^{\sum_n C_n = N} \sum_{m_1=0}^{C_1} \dots \sum_{m_N=0}^{C_N} \gamma_1^{\sum_n m_n}(\beta) \prod_{n=1}^N \frac{\xi_n^{C_n - m_n}(\beta)}{m_n! (C_n - m_n)! n^{C_n}}, \quad (39)$$

where we have used the factorization property of the ground-state contribution (37), which reads $\gamma_n(\beta) = \gamma_1^n(\beta)$.

Now we are able to determine the weight of the particles residing in the ground state. Consider first the cases of $N=2$ and $N=3$ particles, where (39) yields

$$Z_2^B = \gamma_1^0 \frac{1}{2} (\xi_1^2 + \xi_2) + \gamma_1^1 \xi_1 + \gamma_1^2, \quad (40)$$

$$Z_3^B = \gamma_1^0 \left(\frac{1}{6} \xi_1^3 + \frac{1}{2} \xi_1 \xi_2 + \frac{1}{3} \xi_3 \right) + \gamma_1^1 \frac{1}{2} (\xi_1^2 + \xi_2) + \gamma_1^2 \xi_1 + \gamma_1^3. \quad (41)$$

This can, of course, be directly obtained from (10) and (11) by inserting the decomposition (36). The number of particles in the ground state coincides always with the power of γ_1 . Thus, the ground-state weights W_2^B and W_3^B associated with Z_2^B and Z_3^B are

$$W_2^B = 0 \times \gamma_1^0 \frac{1}{2} (\xi_1^2 + \xi_2) + 1 \times \gamma_1^1 \xi_1 + 2 \times \gamma_1^2, \quad (42)$$

$$W_3^B = 0 \times \gamma_1^0 \left(\frac{1}{6} \xi_1^3 + \frac{1}{2} \xi_1 \xi_2 + \frac{1}{3} \xi_3 \right) + 1 \times \gamma_1^1 \frac{1}{2} (\xi_1^2 + \xi_2) + 2 \times \gamma_1^2 \xi_1 + 3 \times \gamma_1^3. \quad (43)$$

The general formula for the weight of the particles in the ground state is therefore given by

$$W_N^B(\beta) = \sum_{C_1, \dots, C_N}^{\sum_n C_n = N} \sum_{m_1=0}^{C_1} \dots \sum_{m_N=0}^{C_N} \left(\sum_{n=1}^N n m_n \right) \times [\gamma_1(\beta)]^{\sum_n m_n} \prod_{n=1}^N \frac{\xi_n^{C_n - m_n}(\beta)}{m_n! (C_n - m_n)! n^{C_n}}. \quad (44)$$

B. Recursion relation

The evaluation of the cycle representation (44) of the ground-state weight is quite cumbersome for large particle

numbers N . Thus, we aim at deriving a more efficient relation for determining $W_N^B(\beta)$. Therefore, we observe that the canonical partition function (39) and the ground-state weight (44) are related via

$$W_N^B(\beta) = \gamma_1(\beta) \frac{\partial}{\partial \gamma_1(\beta)} Z_N^B(\beta). \quad (45)$$

It is useful to define a generating function for the ground-state weight as the sum

$$\mathcal{W}_{\text{GC}}^B(\beta, z) = \sum_{N=0}^{\infty} W_N^B(\beta) z^N, \quad (46)$$

from which we conclude with Eqs. (21) and (45)

$$\mathcal{W}_{\text{GC}}^B(\beta, z) = \gamma_1(\beta) \frac{\partial}{\partial \gamma_1(\beta)} Z_{\text{GC}}^B(\beta, z). \quad (47)$$

Taking into account the decomposition (36) we see that according to (25),

$$\mathcal{W}_{\text{GC}}^B(\beta, z) = Z_{\text{GC}}^B(\beta, z) \sum_{n=1}^{\infty} \gamma_n(\beta) z^n. \quad (48)$$

The canonical ground-state weights can then be found according to Eq. (46) as the Taylor coefficients following from

$$\begin{aligned} W_N^B(\beta) &= \frac{1}{N!} \left. \frac{\partial^N \mathcal{W}_{\text{GC}}^B(\beta, z)}{\partial z^N} \right|_{z=0} \\ &= \sum_{l=1}^N \frac{1}{l! (N-l)!} \left. \frac{\partial^{N-l} Z_{\text{GC}}^B(\beta)}{\partial z^{N-l}} \right|_{z=0} \sum_{n=1}^{\infty} \gamma_n(\beta) \left. \frac{\partial^l z^n}{\partial z^l} \right|_{z=0}. \end{aligned} \quad (49)$$

Using Eqs. (22) and (29), we obtain the canonical ground-state weights as

$$W_N^B(\beta) = \sum_{n=1}^N \gamma_n(\beta) Z_{N-n}^B(\beta), \quad (50)$$

which represents the result of Ref. [15]. It states that the weight $W_N^B(\beta)$ of the particles residing in the ground state of an N -particle Bose gas is immediately known, once the canonical partition functions $Z_n^B(\beta)$ are calculated for all $n < N$. A proper normalization of the statistical ground-state weight $W_N^B(\beta)$ allows us to determine the probability $w_N^B(\beta)$ to find a particle in the ground state,

$$w_N^B(\beta) = \frac{W_N^B(\beta)}{N Z_N^B(\beta)}. \quad (51)$$

This quantity multiplied by N represents the condensed fraction N_0 of an N -particle bosonic ensemble.

VII. SPECIAL POTENTIALS

Now we specify the potential energy $V(\mathbf{x})$ and calculate the heat capacity and the ground-state occupancy within canonical ensembles. In order to see what can go wrong, we first follow Feynman's textbook on statistical mechanics [10] and describe in Sec. VII A the homogeneous Bose gas,

which leads to unphysical results. This is corrected in Sec. VII B by a modified approach for the homogeneous gas where the special role of the ground state is properly taken into account. This approach corresponds to the semiclassical treatment of a Bose gas in a boxlike trapping potential, which is then investigated quantum mechanically exact in Sec. VII C.

Although the quantities of interest may be calculated in principle analytically from Eqs. (30) and (50), the calculations in this section are performed numerically with a C-program in order to reach large particle numbers. More details concerning analogous numerical implementation techniques are presented in Ref. [19].

A. Homogeneous Bose gas

Consider a gas of noninteracting bosons without any trapping potential, $V(\mathbf{x})=0$, i.e., the homogeneous Bose gas. This theoretical model represents a paradigm studied in the seminal work by Bose and Einstein [23]. Also the original work of Feynman [10] within the canonical ensemble relies on treating the homogeneous Bose gas. But this historical important model has problems, which manifest themselves in a divergent ground-state occupancy and in a violation of the third law of thermodynamics. To exhibit this explicitly, we insert the free-particle energies

$$E_{\mathbf{k}} = \frac{\hbar^2}{2M} \mathbf{k}^2 \quad (52)$$

with continuous wave vectors \mathbf{k} into the one-particle partition function (32) and perform the sum over all energy levels in the form of a continuous integral,

$$\sum_{\mathbf{k}} \rightarrow V \int \frac{d^3 k}{(2\pi)^3}, \quad (53)$$

with V being the volume of the system. The result is

$$Z_1(n\beta) = \frac{V}{\lambda^3} \frac{1}{n^{3/2}}, \quad (54)$$

where $\lambda = \sqrt{2\pi\beta\hbar^2/M}$ denotes the thermodynamic de Broglie wavelength. According to (52) the ground-state energy vanishes for the homogeneous case, thus leading to the ground-state contribution (37) of the partition function

$$\gamma_1(n\beta) = 1, \quad (55)$$

which is independent of temperature. Now we use a dimensionless temperature parameter

$$\tau = V^{2/3} \frac{k_B M}{2\pi\hbar^2} T \quad (56)$$

and represent our results for one and two particles. From recursion relation (30) we obtain the canonical partition functions

$$Z_1^B(\tau) = \tau^{3/2}, \quad Z_2^B(\tau) = \frac{\tau^{3/2}}{2^{5/2}} + \frac{\tau^3}{2}, \quad (57)$$

which also follow from (10) and (11) with (54). From (57) we calculate the heat capacity according to the thermody-

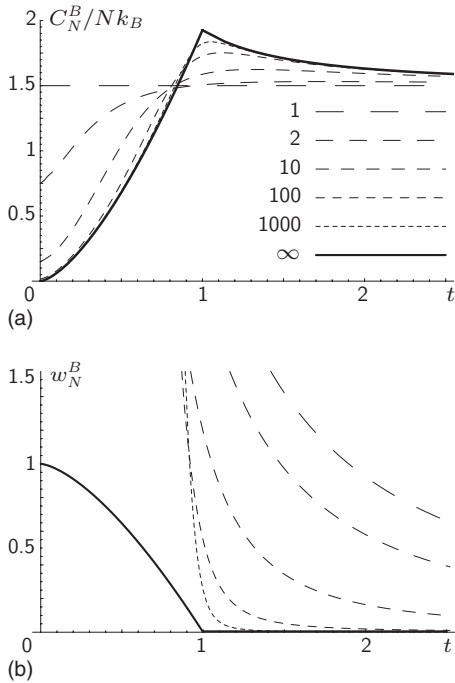


FIG. 3. (a) Heat capacity per particle and (b) ground-state occupancy versus reduced temperature in canonical ensembles of $N = 1, 2, 10, 100, 1000$ particles (dashed lines) compared with the grand-canonical result in the thermodynamic limit (solid line). The particle density is chosen to be constant.

namic equation (31). Using again the dimensionless temperature parameter (56) yields for one and two particles

$$C_1^B(\tau) = \frac{3}{2} k_B, \quad C_2^B(\tau) = 3k_B \frac{1 + 9\sqrt{2}\tau^{3/2} + 16\tau^3}{2 + 8\sqrt{2}\tau^{3/2} + 16\tau^3}. \quad (58)$$

From both results we read off that they obey in the high-temperature limit the classical Dulong-Petit law $C_N^B \rightarrow 3Nk_B/2$. However, in the small-temperature regime one obtains the general result $C_N^B \rightarrow 3k_B/2$. This finding violates the third law of thermodynamics, according to which the heat capacity must vanish at zero temperature. Both results in (58) are plotted in Fig. 3(a) versus the reduced temperature $t \equiv T/T_c$, where

$$T_c = \frac{2\pi\hbar^2}{k_B M} \left(\frac{N}{V\zeta(3/2)} \right)^{2/3} \quad (59)$$

represents the critical temperature of an ideal homogeneous Bose gas. The reduced temperature t is related to τ of Eq. (56) by

$$t = \left(\frac{\zeta(3/2)}{N} \right)^{2/3} \tau. \quad (60)$$

In order to obtain results for larger particle numbers, we evaluate the recursion relation (30). Here the variable (56) is more useful than the reduced temperature (60) since the latter depends explicitly on the particle number. The recursion (30) involves results for different particle numbers, so that the employment of the reduced temperature t would require a

permanent rescaling. Plotting our results for different particle numbers in Fig. 3(a) then only requires a rescaling of the original variable τ to the reduced temperature t according to (60).

This plot shows the behavior of the heat capacity per particle for different total particle numbers. Here, the well-known grand-canonical result is reached in the thermodynamic limit. Furthermore, the heat capacity per particle is suppressed at zero temperature in the thermodynamic limit, but, as mentioned before, the heat capacity itself remains nonvanishing for $t=0$.

A related but much more dramatic problem arises for the homogeneous Bose gas in finite systems when we consider the probability to find a particle in the ground state. To illustrate this we calculate first from (50) the ground-state weights for one and two particles using (55)

$$W_1^B(\tau) = 1, \quad W_2^B(\tau) = 1 + \tau^{3/2}, \quad (61)$$

which also follows from (42) and (43). The ground-state probability (51) then yields with (57) and (61),

$$w_1^B(\tau) = \frac{1}{\tau^{3/2}}, \quad w_2^B(\tau) = \frac{2\sqrt{2}}{\tau^{3/2}} \frac{1 + \tau^{3/2}}{1 + 2\sqrt{2}\tau^{3/2}}. \quad (62)$$

Here we see that the probability to find a particle in the ground state decays for increasing temperature but diverges for low temperatures. This behavior is depicted in Fig. 3(b) where the ground-state occupancy is also shown for larger particle numbers. One can also see that our canonical results do not match the well-known grand-canonical shapes in the thermodynamic limit. Moreover, it diverges for all finite systems at zero temperature. Not only that this divergence is physically meaningless, but by definition any probabilities must be bounded by unity. In the present description of the homogeneous Bose gas in the canonical ensemble this is obviously not the case. As it will be seen in the next section, this problem appears due to an improper treatment of the semiclassical limit and the results can be corrected by taking care of the special role of the ground state.

B. Homogeneous Bose gas with ground state

Inspecting the results in the preceding section more carefully, we recognize already at the beginning a contradiction between the one-particle partition function (54) and its ground-state contribution (55). Namely, whereas (54) vanishes for low temperatures, the ground-state partition remains finite. This leads to a negative contribution for all excited states. However, one would reasonably expect that the latter must be always positive and vanishes only for zero temperature. According to this expectation we suppose that the partition function must be a sum of the ground-state contribution (55) and the contribution of excited states in the form given by (54),

$$Z_1(n\beta) = 1 + \frac{V}{\lambda^3} \frac{1}{n^{3/2}}. \quad (63)$$

Such a decomposition is equivalent to replace condition (53) by

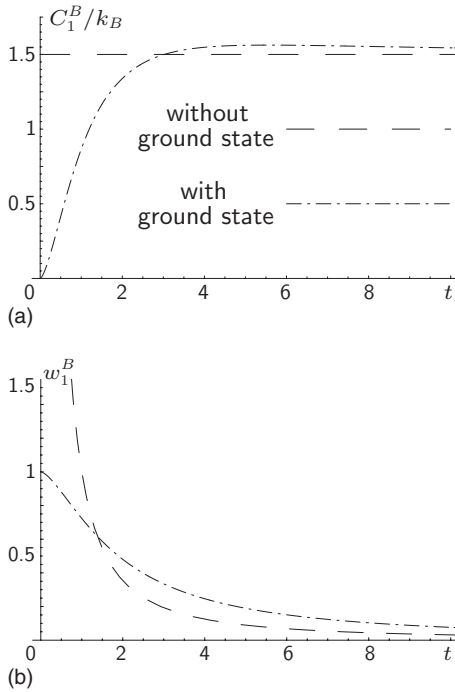


FIG. 4. (a) Heat capacity and (b) ground-state probability for one particle versus reduced temperature calculated without (dashed line) and with an extra ground state (dashed-dotted line).

$$\sum_{\mathbf{k}} f(\mathbf{k}) \rightarrow f(0) + V \int \frac{d^3k}{(2\pi)^3} f(\mathbf{k}) \quad (64)$$

for any function $f(\mathbf{k})$. Comparing (64) with relation (53) we see that the ground state in the latter did not play any special role. There we integrated over all states including the ground state, so that the latter was only a point of zero measure, as was basically any other state. In our present approach, however, we separate the ground state explicitly from the remaining excited states. In order to demonstrate how well this procedure works, we calculate the heat capacity (31) of one particle from (63), yielding for $D=3$ spatial dimensions

$$C_1^B(\tau) = \frac{3k_B}{2} \frac{5\tau^{3/2} + 2\tau^3}{2 + 4\tau^{3/2} + 2\tau^3}. \quad (65)$$

This leads to $3k_B/2$ in the high-temperature limit according to the Dulong-Petit law. For small temperatures the heat capacity (65) vanishes satisfying also the third law of thermodynamics. Both results (58) and (65) for the heat capacity of one particle are compared in Fig. 4(a).

The second problem of the homogeneous Bose gas in the preceding section concerns the probability to find a particle in the ground state which diverges for vanishing temperature. Taking into account the extra ground state, we recognize that (55) represents its contribution to the partition function (63). Thus, the probability for a particle to be in the ground state seems to be normalized. For one particle we use Eq. (50) to obtain $W_1^B(\tau) = \gamma_1(\tau)$, yielding with the definition (51) the ground-state probability

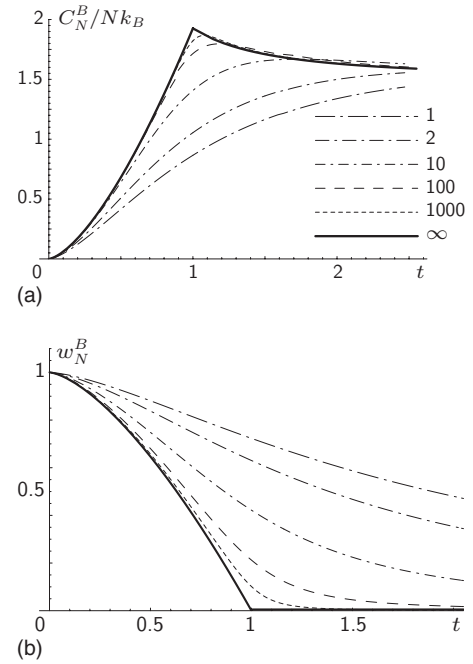


FIG. 5. (a) Heat capacity per particle and (b) ground-state occupancy versus reduced temperature calculated with an extra ground state according to (63). Results are represented for canonical ensembles of $N=1,2,10,100,1000$ particles (dashed and dashed-dotted curves) and for the grand-canonical ensemble in thermodynamic limit (solid curve) for a fixed particle density.

$$w_1^B(\tau) = \frac{1}{1 + \tau^{3/2}}. \quad (66)$$

It vanishes for high temperature ($\tau \gg 1$) and has its maximal value of 1 for zero temperature, as one may expect on general physical grounds. We compare this result with the corresponding one of the preceding section in Fig. 4(b). For small temperatures the corrected curve does not diverge and shows the expected behavior. One understands immediately, why this procedure works so well for finite systems. Assuming the particle density to be equal for all systems, the volume V must be small for small particle numbers. The additional unity in (63) plays for them a more important role than for larger ensembles. Moreover, this unity is practically negligible for high enough temperatures and carries a larger weight for lower temperatures. As the contributions of different lower particle numbers are mixed in the quantities of interest (30) and (50), this influences the situation decisively.

Now we turn to many-body systems and calculate their heat capacity according to the recursion relation (30) with definition (31) and the ground-state probability according to (50) with (51). The corresponding results are represented in Fig. 5. All curves have the correct behavior for high temperatures as well as for the low-temperature region. Moreover, in the thermodynamic limit, where the particle number goes to infinity, both results display the grand-canonical shape. This means that, although all curves are smooth for finite systems, the behavior of the heat capacity and the ground-state occu-

pancy change more pronounced at the critical point by increasing the number of particles.

Thus, we can summarize that a careful treatment of the ground state in this section improves the description of the homogeneous Bose gas in a fundamental way. Nevertheless, also this attempt represents only a physical approximation to a real finite system. To this end we will show in the next section that the exact quantum-mechanical results deviate quantitatively in a significant way from the semiclassical treatment presented here.

C. Bose gas in a box potential

In this section we work out the exact quantum-mechanical treatment of a Bose gas in a square box potential. For convenience, we choose the size of our box to be equal to L in all spatial directions, so that the trapping potential reads

$$V(\mathbf{x}) = \begin{cases} 0, & 0 \leq x_j \leq L \quad \text{for all } j = 1, 2, 3, \\ \infty, & \text{elsewhere.} \end{cases} \quad (67)$$

The one-particle Schrödinger equation is then solved exactly by the energy eigenvalues

$$E_{\mathbf{k}} = \frac{\pi^2 \hbar^2}{2ML^2} \mathbf{k}^2 \quad \text{with } k_j = 1, 2, 3, 4, \dots \quad (j = 1, 2, 3). \quad (68)$$

As one can deduce from the normalization condition of the eigenstates, the value $\mathbf{k} = (k_1, k_2, k_3)$ is not a solution, if at least one k_j vanishes. Thus, the ground-state energy is given by $E_G = 3\pi^2 \hbar^2 / (2ML^2)$. From this we obtain the ground-state contribution to the partition function (37) which reads with the dimensionless temperature parameter (56) as

$$\gamma_1(n\beta) = e^{-3n\pi/(4\tau)}. \quad (69)$$

The one-particle partition function then reads

$$Z_1(n\beta) = \left(\sum_{m=1}^{\infty} e^{-n\pi m^2/(4\tau)} \right)^3. \quad (70)$$

The corresponding quantities in Secs. VII A and VII B are different semiclassical approximations of (69) and (70), which are justified for an infinitely large box. Such a semiclassical approximation leads, at first, to the ground-state contribution (55) and, second, to a vanishing level spacing which gives rise to the continuously distributed energy levels (52). Therefore, the sum in (70) must be replaced by an integral according to (53) or (64), respectively. The one-particle partition function is then given by a Gaussian integral and can be simply calculated leading to (54) or (63). Strictly speaking, this semiclassical description of a finite system is inadequate insofar as it is impossible to have a finite number of particles in an infinite box, unless in the trivial case of zero density.

The partition function (70) in a box cannot be calculated exactly. Thus, we can evaluate the sum only approximately up to a certain order of the summation index m . However, this procedure does not work well for all temperatures since the exponential functions $e^{-n\pi m^2/(4\tau)}$ in (70) are required to be small, and this is only true for small temperatures ($\tau \ll 1$). In

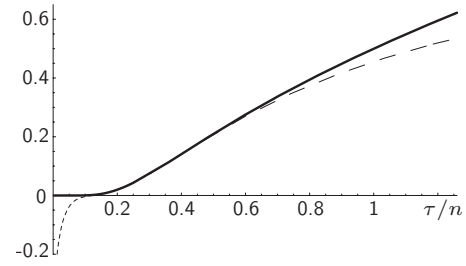


FIG. 6. Comparison between the exact sum $\sum_{m=1}^{\infty} e^{-n\pi m^2/(4\tau)}$ (solid line) and their lowest small-temperature approximation $e^{-n\pi/(4\tau)}$ (long dashed curve) according to (70) and the lowest high-temperature approximation $\sqrt{\tau/n} - 1/2 + 2\sqrt{\tau/n} e^{-4\pi\tau/n}$ (short dashed curve) from (72).

order to perform the sum in (70) also for high temperatures, we need its dual expression, which follows from the Poisson summation formula [11]

$$\sum_{m=-\infty}^{\infty} f(m) = \sum_{q=-\infty}^{\infty} \int_{-\infty}^{\infty} dz f(z) e^{2\pi i q z}. \quad (71)$$

With this, the one-particle partition function (70) is converted into

$$Z_1(n\beta) = \left(\sqrt{\frac{\tau}{n}} - \frac{1}{2} + 2\sqrt{\frac{\tau}{n}} \sum_{q=1}^{\infty} e^{-4\pi\tau q^2/n} \right)^3. \quad (72)$$

Of course, this function cannot be calculated exactly either, so we must perform the summation here also only up to a certain order. Whereas the approximation (70) is applicable for small temperatures, its dual (72) can be evaluated for high temperatures. How can we now use both representations (70) and (72) in order to evaluate the one-particle partition function in the whole temperature range? In principle, both representations are equivalent, but only when both series are evaluated exactly. This exact expression is approximated well by summing a few terms in (70) only below a certain temperature and in (72) only above a certain temperature. There exists an appropriate temperature region where both approximations coincide. In Fig. 6 we see that for the interval $0.1 < \tau/n < 0.5$ even the lowest term in (70) as well as (72) are sufficient. By taking more terms into account, this matching region grows. For practical calculations, however, the summation of many terms costs much effort, so it is more efficient to precisely define an intermediate temperature, which joins the low-temperature region with the high-temperature region best.

In order to calculate the results for many particles we use the recursion relation (30) for the partition functions and (50) for the ground-state weights. The heat capacity is then calculated from (31) and the ground-state occupancy from (51). Results for $N=1, 2, 10, 100, 1000$, and $10\,000$ bosons are depicted in Fig. 7. All results for the heat capacity exhibit the Dulong-Petit behavior in the high-temperature limit and fulfill the third law of thermodynamics for $T \rightarrow 0$. The ground-state occupancy is 100% for zero temperature and vanishes for high temperatures. One specific feature of an

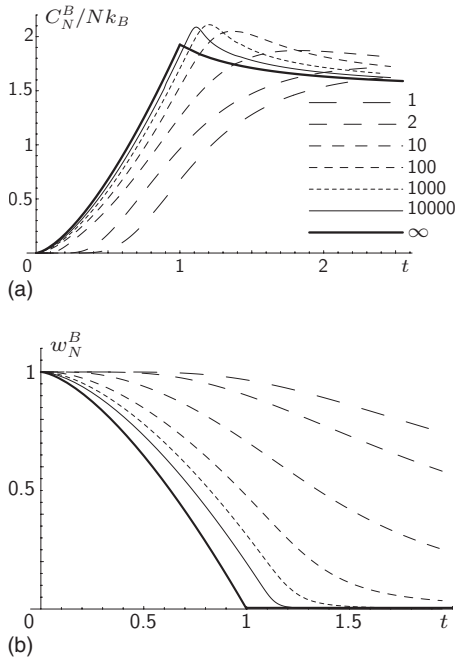


FIG. 7. (a) Heat capacity per particle and (b) ground-state occupancy versus reduced temperature in the exact square box potential for ensembles of $N=1, 2, 10, 100, 1000, 10\,000$ bosons (dashed and thin curves) and in the grand-canonical ensemble in the thermodynamic limit (thick solid curve). All results are calculated for the same particle density.

exact quantum-mechanical treatment is worth emphasizing. Due to the nonvanishing gap between the ground state and the first excited state, the slope of the heat capacity is exponential for small temperatures. This is especially visible for small particle numbers N . For higher N , the exponential region decreases and is followed by the usual power-law increase $\sim t^{3/2}$. In the thermodynamic limit the exponential region disappears and the power behavior takes over.

As expected, the canonical results converge in the thermodynamic limit toward the grand-canonical one for an infinite average particle number. However, this convergence is much slower in the quantum-mechanical exact treatment than in the semiclassical approximation of the preceding section. This manifests itself, for instance, in an apparent discrepancy in the location and extent of the heat capacity maximum even for $N=10\,000$ particles. The same observation holds for the ground-state occupancy. Although an increase of the particle number makes the curves sharper in the crossover region, the location of the latter is clearly shifted toward higher temperatures. This gives rise to the so-called finite-size effect which will be elaborated in the subsequent section.

VIII. FINITE-SIZE EFFECT

Let us now investigate in detail the crossover temperature, which can be regarded as a generalized critical temperature T_c . At first, we suggest to define this as the temperature where the ground-state occupancy possesses the largest cur-

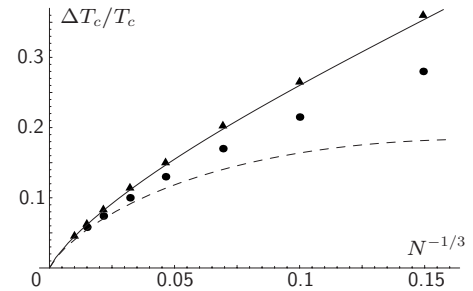


FIG. 8. Shifts of critical temperature for N bosons in a square box potential with $N=300, 1000, 3000, 10\,000, 30\,000, 100\,000, 300\,000$ (from the right-hand to the left-hand side) in the canonical ensemble (dots). They differ considerably from the grand-canonical results (triangles) with the same boson numbers. The dashed curve corresponds to the semiclassical result (73) within the grand-canonical ensemble from Ref. [25]. The solid curve represents our result $\Delta T_c / T_c = t_c - 1$ according to Eq. (83).

vature. This definition is motivated by the fact that in the thermodynamic limit this quantity has an infinite curvature at the critical point. By analogy, in a finite ensemble the point with a significantly sharp rise in the curvature may play the role of the transition temperature. These points are plotted with dots in Fig. 8 for different particle numbers. The finite-size effects are quite large. In a box confinement, they amount to 30% for $N=300$ and to about 5% for $N=300\,000$ bosons. The effects here are from 3 to 4 times larger than for the Bose gas confined in a harmonic trap [4]. Furthermore, it is remarkable that the finite-size shifts of T_c point upwards which is opposite to the harmonic case. This fact can be explained by a stability analysis, which shows that in a three-dimensional box potential only finite systems are stable [24]. Particle fluctuations grow with the size of the box, resulting in a loss of stability, and this is why bigger systems condense at lower temperatures.

Let us compare our canonical results for the critical temperature with analytic approximations. The first estimate of the shift of the critical temperature was given in Ref. [25] by

$$\frac{\Delta T_c}{T_c} = \frac{1}{\zeta^{2/3}(3/2)N^{1/3}} \ln \left(\frac{4N^{2/3}}{3\pi\zeta^{2/3}(3/2)} \right) + \dots \quad (73)$$

This result is plotted in Fig. 8 as a dashed curve. It represents the grand-canonical result for semiclassical corrections caused by large but finite particle numbers N , which takes into account the nonvanishing energy eigenvalues k_j of (68) in a box potential. This correction was calculated in Ref. [25] by replacing the sum over all energy eigenstates in (35) by a momentum integration and subtracting all states lying at coordinate planes in the momentum space. As one can see in Fig. 8, this analytic result reproduces well the direction of the critical temperature shift but drastically underestimates its magnitude. Further corrections could be obtained by avoiding the double counting at cross sections of coordinate planes as well as by taking into account the finite gap between the ground state and the first excited states.

Here we prefer a more controllable procedure for calculating the finite-size corrections which goes as follows. We

start with the cycle number representation of the grand-canonical average of the particle number according to Eqs. (25) and (35),

$$\langle N \rangle = \sum_{n=1}^{\infty} Z_1(n\beta) z^n = \langle N_0 \rangle + \langle N_T \rangle. \quad (74)$$

It contains the number of particles in the ground-state condensate

$$\langle N_0 \rangle = \sum_{n=1}^{\infty} e^{-n\beta E_G} z^n = \frac{1}{z^{-1} e^{\beta E_G} - 1} \quad (75)$$

and the number of thermal particles in excited states

$$\langle N_T \rangle = \sum_{n=1}^{\infty} [Z_1(n\beta) - e^{-n\beta E_G}] z^n. \quad (76)$$

Furthermore, we rewrite the one-particle partition function (70) as

$$Z_1(n\beta) = e^{-3n\pi/(4\tau)} [1 + e^{-3n\pi/(4\tau)} \sigma(\pi/n)]^3 \quad (77)$$

with dimensionless temperature (56) and an excitation contribution

$$\sigma(\tau) = \sum_{m=2}^{\infty} e^{-\pi(m^2-4)/(4\tau)} = \sqrt{\tau} - 3/2 + \pi/\sqrt{\tau} + O(1/\tau), \quad (78)$$

where the latter equation is the high-temperature approximation similar to the duality relation (72) for the whole partition function. Since we aim at finding the location of the critical temperature, we demand for the fugacity z the condition $z e^{-\beta E_G} = z e^{-3\pi/(4\tau)} \approx 1$ but at the same time $\langle N_0 \rangle \ll \langle N \rangle$. Both conditions are exactly fulfilled in the thermodynamic limit and are reasonable approximations for large but finite systems. From Eqs. (74)–(78) we obtain at the critical point $\tau = \tau_c$ approximately

$$\langle N \rangle = \sum_{n=1}^{\infty} [3e^{-3n\pi/(4\tau_c)} \sigma(\tau_c/n) + 3e^{-6n\pi/(4\tau_c)} \sigma^2(\tau_c/n) + e^{-9n\pi/(4\tau_c)} \sigma^3(\tau_c/n)]. \quad (79)$$

According to Eq. (78) the sums in (79) can be expanded in terms of the polylogarithmic Bose functions $\zeta_\nu(e^{-x}) \equiv \sum_{n=1}^{\infty} e^{-nx}/n^\nu$ as

$$\begin{aligned} \langle N \rangle &= \tau_c^{3/2} \zeta_{3/2}(e^{-9\pi/(4\tau_c)}) + \frac{3\tau_c}{2} [2\zeta_1(e^{-6\pi/(4\tau_c)}) - 3\zeta_1(e^{-9\pi/(4\tau_c)})] \\ &+ \frac{3\tau_c^{1/2}}{4} [4\zeta_{1/2}(e^{-3\pi/(4\tau_c)}) - 12\zeta_{1/2}(e^{-6\pi/(4\tau_c)}) \\ &+ (4\pi + 9)\zeta_{1/2}(e^{-9\pi/(4\tau_c)})] + \dots \end{aligned} \quad (80)$$

For large values of τ_c , the polylogarithmic functions are evaluated with the help of the Robinson formula [26]

$$\zeta_\nu(e^{-x}) = \begin{cases} \Gamma(1-\nu)x^{\nu-1} + \sum_{k=0}^{\infty} (-x)^k \zeta(\nu-k)/k! & \text{for } 1 \neq \nu < 2, \\ -\ln x + \sum_{k=1}^{\infty} (-x)^k \zeta(1-k)/k! & \text{for } \nu = 1, \end{cases} \quad (81)$$

where $\Gamma(z)$ denotes the Γ function and $\zeta(z) \equiv \sum_{n=1}^{\infty} 1/n^z$ denotes the Riemann ζ function. Inserting this into (80) and identifying $\langle N \rangle$ with the actual particle number N , we arrive at

$$\begin{aligned} N &= \tau_c^{3/2} \zeta(3/2) + \frac{3}{2} \tau_c \ln \left(C_3 \frac{\pi}{2\tau_c} \right) + \frac{3(\pi+1)}{4} \tau_c^{1/2} \zeta(1/2) \\ &+ O(\tau_c^0). \end{aligned} \quad (82)$$

Using the reduced temperature $t \equiv T/T_c$ instead of τ according to (60), this can also be rewritten as

$$\begin{aligned} t_c^{3/2} &= 1 + \frac{3}{2} \frac{t_c}{N^{1/3} \zeta^{2/3}(3/2)} \ln \left(\frac{2N^{2/3}}{\pi \zeta^{2/3}(3/2) C_3} \frac{t_c}{C_3} \right) \\ &- \frac{3(\pi+1)}{4} \frac{t_c^{1/2} \zeta(1/2)}{N^{2/3} \zeta^{1/3}(3/2)} + O(1/N). \end{aligned} \quad (83)$$

Taking into account only the first term on the right-hand side yields the semiclassical result $t_c = 1$. The first correction involves a coefficient C_3 which unfortunately cannot be calculated directly. The origin of this problem is the divergence of the polylogarithmic function $\zeta_\nu(z)$ for $z \approx 1$ and any $\nu \leq 1$, which is explicitly given by the first term in (81). So one can see that the last three terms in Eq. (80) contribute not only to the order of $\tau_c^{1/2}$ but also to the order τ_c . The same is valid for all other terms which we omitted in (80). The leading finite-size correction of τ_c plays here a special role insofar as it consists of infinitely many terms and thus its factor C_3 cannot be calculated from the first few terms. However, we can perform a direct numerical evaluation, yielding the value $C_3 \approx 0.9574$ which also follows from a semianalytic calculation [11]. In contrast to that, all higher corrections in (83) are analytically calculable.

In fact, such a problem is not typical for the box potential only. In a harmonic trap, one encounters an analogous situation for the subleading finite-size correction instead of the leading one for the present box case. Here, we should mention, that it is just this nonanalyticity of the leading finite-size effect, which is responsible for the failure of the approximation in Ref. [25], see Eq. (73) here. Their perturbative approach yielded the factor 3/2 instead of the numerical correct C_3 value.

By extracting the N dependence of the reduced critical temperature of Eq. (83), we now obtain a grand-canonical semiclassical result which is represented by the solid line in Fig. 8. As one can see, it overestimates canonical results considerably. In fact, although many physical properties within canonical and grand-canonical ensemble are equal in the thermodynamic limit, they can be quite different for finite

systems. Let us now determine crossover temperatures for finite grand-canonical ensembles in the same way as before in the canonical approach. To this end we calculate the ground-state occupancy for a grand-canonical system. As already outlined at the beginning of Sec. VI, this is done by determining at first the fugacity z which corresponds to a given average particle number $\langle N \rangle$ for a fixed temperature from (74) and inserting its value into (75). The resulting quantity $\langle N_0 \rangle / \langle N \rangle$ is a smooth function of temperature similar to the canonical results in Fig. 7(b) but somewhat shifted to the right-hand side. The crossover temperatures are then calculated by analogy with the canonical case as points of largest curvature and are indicated by solid triangles in Fig. 8. They agree very well with the analytic approximation of (83) even for smaller systems of a few hundred particles, but differ strongly from canonical values.

It is well known that the canonical partition function can be obtained from the grand-canonical partition function by means of the integral over the chemical potential μ using the identity

$$Z_N^B = \beta \int_{c-i\infty}^{c+i\infty} \frac{d\mu}{2\pi i} e^{-\beta\mu N} Z_{GC}^B(\mu). \quad (84)$$

In the leading saddle-point or steepest-descent approximation one obtains

$$\ln Z_N^B = \ln Z_{GC}^B(\bar{\mu}) - \beta\bar{\mu}N + \dots, \quad (85)$$

where $\bar{\mu}$ is the extremal point of the exponent $-\beta\mu N + \ln Z_{GC}^B(\mu)$ in (84). The extremity condition implies by means of Eq. (34) immediately the usual Bose-Einstein distribution (35). For infinite N , this approximation becomes exact, leading to the equality of thermodynamical properties [1,27] in canonical and grand-canonical ensembles.

For finite N , one may want to calculate corrections from the neighborhood of the saddle point. The naive perturbation up to first order, however, yields a wrong sign of the shift for the critical temperature. A detailed analysis shows that a nonanalyticity occurs at the saddle point near the critical point and infinitely many orders in the saddle point expansion must be calculated and resummed to find the correct result. This fact has been discussed in the literature, for instance, in [1] for the box potential and in [28] for a general case near the critical point, and is not yet solved.

IX. CONCLUSION

By taking into account the special role of the ground state of the system, we have obtained a consistent semiclassical description of an ideal Bose gas of a fixed finite number of particles confined in a box. We have thus improved Feynman's original canonical approach for treating the ideal homogeneous Bose gas. Finite-size effects have been shown to be significant, even for a moderate number of particles. Our canonical findings are compared with grand-canonical ones, for which we have found analytic expressions which improve results in the literature. An analogous analytic expression within the canonical ensemble could not be found, so we must be content with numerical results, which were given in the present paper.

Our canonical investigation may serve as a theoretical basis for future experiments in boxlike traps manufactured with strongly inhomogeneous fields or laser beams.

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