Microcanonical fluctuations of a Bose system's ground state occupation number

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Employing asymptotic formulas from the partition theory of numbers, we derive the microcanonical probability distribution of the ground state occupation number for a one-dimensional ideal Bose gas confined at low temperatures by a harmonic potential. We compare the grand canonical analysis to the microcanonical one, and show how the fluctuation catastrophe characteristic for the grand canonical ensemble is avoided by the proper microcanonical approach. [S1063-651X(96)06210-1]

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The recent groundbreaking work on Bose-Einstein condensation of trapped alkali-metal atoms [1–3] forces us to rethink some all-too-familiar concepts. Conventionally, the statistical theory of ideal Bose gases is based on the grand canonical ensemble: the given system is assumed to be in contact with a particle-energy reservoir. The mean occupation number, at temperature T, of a single-particle state with energy ε_j is

$$\langle n_j\rangle = \frac{1}{\exp[(\varepsilon_j-\mu)/kT]-1}, \tag{1}$$

where k is Boltzmann's constant. The chemical potential μ is fixed by the requirement that the sum of all $\langle n_j\rangle$ yields the preassigned average number of particles $\langle N\rangle$:

$$\sum_j \langle n_j\rangle = \langle N\rangle. \tag{2}$$

The occupation numbers of the single-particle states fluctuate, both because there are transitions between the states, and because the system exchanges particles with the reservoir. The relative mean square fluctuations are given by [4]

$$\frac{\langle n_j^2\rangle - \langle n_j\rangle^2}{\langle n_j\rangle^2} = \frac{1}{\langle n_j\rangle} + 1. \tag{3}$$

When the temperature approaches zero, all particles occupy the ground state, so that $\langle n_0\rangle \approx \langle N\rangle$. Then the relative mean square fluctuations of the ground state population, and thus the relative fluctuations of the total particle number, approach unity: as a result of particle exchange with the reservoir, the uncertainty of the number of particles $\langle N\rangle$ comprising the system becomes comparable to $\langle N\rangle$ itself. This fluctuation catastrophe is related to the divergency of the quantum coherence length λ_T for $T\to 0$. When λ_T vastly exceeds the length scale characterizing the system under consideration, a rigid distinction between ''system'' and ''reservoir'' is no longer practical.

Equation (3), while strictly valid in the framework of the grand canonical ensemble [5], is not applicable to a low-temperature Bose gas that does *not* exchange particles with a reservoir. In this case the fluctuations have to vanish for $T\to 0$, when all particles become tied in the ground state. But what is then the behavior of the fluctuations at low temperatures? More precisely, supposing that the gas has a certain total energy, what is the probability density for finding a fraction n_0/N of all particles in the ground state?

In view of the pioneering work on Bose-Einstein condensation of dilute alkali-metal vapors [1–3], these questions are by no means merely academical. On a time scale relevant for these experiments, ultracold atoms stored in their traps do neither *exchange* energy nor particles with a *reservoir* (although atoms *leave* the trap during the process of evaporative cooling), so that the physics should be described by a *microcanonical* approach. Since the different thermodynamical ensembles cannot be considered as equivalent for condensed Bose gases, it is of utmost importance to investigate to which extent the predictions of the conventional grand canonical theory of Bose-Einstein condensation differ from those of the more appropriate microcanonical one.

However, a general microcanonical theory of Bose systems is quite difficult. *Any* particular system which lends itself to a detailed comparison between the microcanonical and the grand canonical approach must be regarded as a real gem. The purpose of this paper is to present such a comparison for a one-dimensional gas of ideal Bosons moving in the potential of a harmonic oscillator with frequency ω [6], i.e., we stipulate that the single-particle energies are given by

$$\varepsilon_j = \hbar\omega(j+1/2), \quad j=0,1,2,\ldots. \tag{4}$$

In this case we can resort to powerful theorems from the asymptotic theory of partitions, and even derive the microcanonical probability distribution for the ground state occupation number n_0. Needless to say, we do not intend to model an actual experiment here; our aim is, rather, to investigate the fluctuations of n_0 for a paradigmatic case. Although our model is only one-dimensional, it is not trivial. We also remind the reader that rigorous studies of one-dimensional Fermi systems, such as the influential works by Tomonaga [7] and Luttinger [8], have led to insights of considerable importance.

Let us first briefly reconsider the canonical approach. Applying standard arguments [4], one obtains

$$\frac{\langle n_0\rangle}{\langle N\rangle} \approx 1 - \frac{kT}{\hbar\omega}\,\frac{g_1(z)}{\langle N\rangle}, \tag{5}$$

where $z^{-1} = \exp[(\varepsilon_0-\mu)/kT]$, and

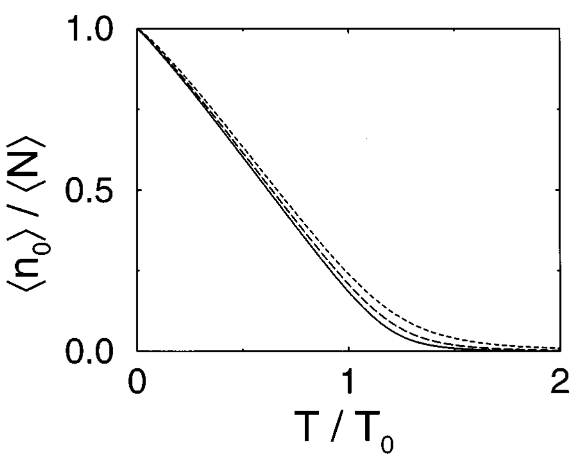

FIG. 1. Grand canonical ground state fractions $\langle n_0\rangle/\langle N\rangle$ versus temperature, for average particle numbers $\langle N\rangle = 10^4$ (short dashes), 10^5 (long dashes), and 10^6 (full line). The characteristic temperature T_0 is defined by $kT_0 = \hbar\omega\langle N\rangle/\ln(\langle N\rangle)$.

$$g_\alpha(z) = \frac{1}{\Gamma(\alpha)}\int_0^\infty \frac{x^{\alpha-1}dx}{z^{-1}e^x - 1}. \tag{6}$$

When the temperature decreases, the chemical potential μ approaches the ground state energy ε_0 from below, so that the fugacity $z = 1/(1+\langle n_0\rangle^{-1})$ approaches unity. Since the Bose function $g_1(z)$ diverges for $z \to 1$, there is no sharp onset of Bose-Einstein condensation for particles in a one-dimensional harmonic oscillator potential [9]. But since this divergency is merely logarithmic, $g_1(z) \sim -\ln(-\ln z) \approx \ln(\langle n_0\rangle)$ for $z \to 1$, and since $\langle n_0\rangle \leqslant \langle N\rangle$ remains bounded, there is still a certain nonzero temperature below which the ground state becomes occupied by a ''macroscopic'' number of particles. This can be seen clearly in Fig. 1, which shows numerically computed grand canonical ground state populations $\langle n_0\rangle/\langle N\rangle$ for $\langle N\rangle = 10^4$, 10^5, and 10^6, as functions of the normalized temperature T/T_0. As motivated by Eq. (5), we have introduced the characteristic temperature

$$T_0 = \frac{\hbar\omega}{k}\frac{\langle N\rangle}{\ln(\langle N\rangle)}. \tag{7}$$

The mean energy $\langle E\rangle$ of the grand canonical system obeys

$$\frac{\langle E\rangle - \langle N\rangle\varepsilon_0}{\hbar\omega} = \left(\frac{kT}{\hbar\omega}\right)^2 g_2(z), \tag{8}$$

with $g_2(z) \approx \pi^2/6$ for $T < T_0$, provided the average number of particles $\langle N\rangle$ is sufficiently large.

The microcanonical analysis is significantly more involved. Given a gas consisting of exactly N particles in a harmonic potential, its total energy is of the form $E = \hbar\omega(m + N/2)$, with integer m. To compute the entropy $S(E,N)$, one has to determine the number of possibilities for distributing the m excitation quanta over the N indistinguishable bosons. For $m \leqslant N$ this is equivalent to determining the number $p(m)$ of partitions of m into an arbitrary number of positive integers. For example, for $m = 4$ there are five partitions, $m = 1+1+1+1$, $m = 2+1+1$, $m = 2+2$, $m = 3+1$, and $m = 4$, which correspond to five different bosonic microstates. The determination of $p(m)$ is a famous problem in combinatorial analysis that had been considered already by Euler [10]; tables with values of $p(m)$ for $m \leqslant 500$ can be found in Ref. [11]. Although even an exact formula for $p(m)$ is available [12], the asymptotic formula derived by Hardy and Ramanujan [13,14] is more suitable for our purposes:

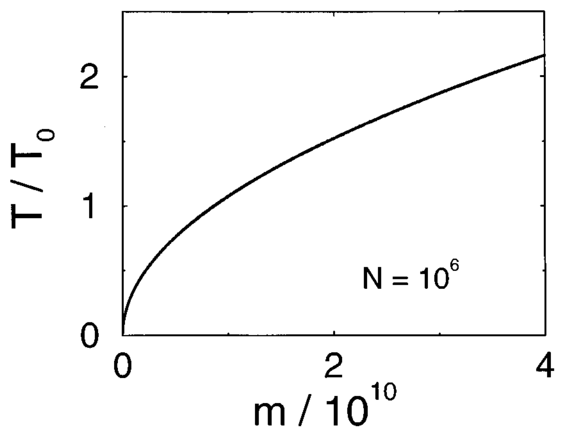

FIG. 2. Microcanonical temperature for $N = 10^6$, versus number m of excitation quanta. This graph is practically indistinguishable from a plot of the corresponding exact grand canonical data, and very well approximated by $T/T_0 = (\hbar\omega/\pi kT_0)\sqrt{6m}$.

$$p(m) \sim \frac{\exp(c\sqrt{m})}{4\sqrt{3}m}, \quad c = \sqrt{\frac{2}{3}}\pi. \tag{9}$$

This formula slightly overestimates the actual value of $p(m)$, but already for $m = 1000$ the error is less than 1.5%.

We then have $S(E,N) = k\ln[p(m)]$ for $m \leqslant N$. If the number m of quanta exceeds the number N of particles, we have to determine the number $p_N(m)$ of partitions of m into *at most N* positive summands. Incidentally, one encounters the very same problem when dealing with the bosonization of one-dimensional Fermions [7,8,15]. There one can argue that for the parameters of interest the restriction on the number of summands yields only an exponentially small correction to $p(m)$, which is then neglected. But in our case the correction to $p(m)$ will become important. Following Erdos and Lehner [16], we have

$$p_N(m) \sim p(m)\exp\left(-\frac{2}{c}\exp[-x_N(m)]\right), \tag{10}$$

where

$$x_N(m) = \frac{cN}{2\sqrt{m}} - \ln(\sqrt{m}). \tag{11}$$

Thus $p_N(m) \approx p(m)$ as long as $\sqrt{m} \ll N$. The entropy now reads $S(E,N) = k\ln[p_N(m)]$, and the microcanonical temperature $T^{(mic)}$ follows from $1/T^{(mic)} = (\partial S/\partial E)_N$. Figure 2 shows the temperature determined in this way versus the number m of quanta for $N = 10^6$. Comparing this plot with the results of a grand canonical calculation for $\langle N\rangle = 10^6$, and with the approximation $T/T_0 \approx (\hbar\omega/\pi kT_0)\sqrt{6m}$ that follows from (8), one finds that on the scale of Fig. 2 all three graphs coincide, i.e., there is no need to distinguish between $T^{(mic)}$ and T.

But the temperature is not very sensitive to possible differences between the ensembles anyway, since it depends merely on the logarithm of the total number of partitions. The ground state occupation number n_0, a quantity of primary experimental interest, is a more sensitive indicator. Let $p(m;r)$ be the number of partitions of m into *exactly* r positive integers. When m is partitioned into r summands ($r \leqslant N$), i.e., when m quanta are distributed over exactly r particles, then there are no quanta left for the remaining $N-r$ particles, so that these have to occupy the oscillator ground state, i.e., $N-r=n_0$. Hence, the probability $w(n_0|m)$ for finding n_0 particles in the ground state when there are m energy quanta is

$$w(n_0|m)=\frac{p(m;N-n_0)}{p_N(m)}. \tag{12}$$

Microcanonically, the expectation value $\overline{n_0}$ of the ground state occupation number is the first moment of $w(n_0|m)$; the fluctuation δn_0 is given by the width of this distribution. (We use the overbar in order to distinguish the microcanonical expectation value $\overline{n_0}$ clearly from its grand canonical counterpart $\langle n_0 \rangle$.)

An asymptotic expression for $p(m;r)$ has been found by Auluck, Chowla, and Gupta [17]:

$$p(m;r) \sim \frac{p(m)}{\sqrt{m}} \exp\left(-\frac{2}{c} \exp[-x_r(m)] - x_r(m) \right), \tag{13}$$

where $x_r(m)$ is defined by (11), with N replaced by r: $x_r(m) = cr/(2\sqrt{m}) - \ln(\sqrt{m})$. Combining (10), (12), and (13), we obtain

$$w(n_0|m) \sim \frac{1}{\sqrt{m}} \frac{\exp\left(-\frac{2}{c} \exp[-x_{N-n_0}(m)] - x_{N-n_0}(m) \right)}{\exp\left(-\frac{2}{c} \exp[-x_N(m)] \right)}. \tag{14}$$

Quite remarkably, $p(m)$ has dropped out of this expression; $w(n_0|m)$ is determined entirely by the correction factors that reflect the respective restrictions on the number of partitions.

This formula (14) remains valid even when the number m of quanta is so large that $x_N(m)$ is slightly negative. In that case the distribution $w(n_0|m)$ is a monotonically decreasing function of n_0. When m becomes smaller, i.e., when the temperature is decreased, $x_N(m)$ becomes positive. For sufficiently large $x_N(m)$ the exponential in the denominator of (14) can be replaced by unity, and $w(n_0|m)$ develops a single maximum for $n_0 \approx N - \sqrt{m}\ln(m)/c$. Together with the known energy-temperature relation, cf. Fig. 2, this distribution now allows us to investigate how the microcanonical fluctuations of the ground state occupation vanish for $T \to 0$.

Figure 3 depicts the shape of $w(n_0|m)$ for $N=10^6$ and various degrees of excitation m, which can be translated into the respective temperatures with the help of Fig. 2. Note that the distribution is not symmetric, so that the expectation value of the ground state occupation number will differ from the most probable value.

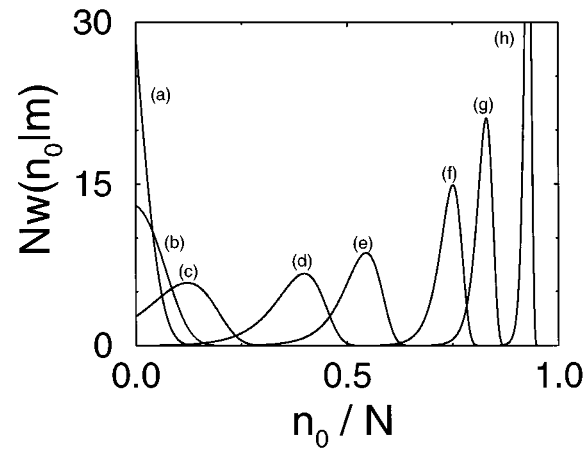

FIG. 3. Microcanonical probability $w(n_0|m)$ for finding n_0 particles in the ground state when the total energy is $E=\hbar\omega(m+N/2)$, multiplied by the total particle number $N=10^6$. The respective values of m (the temperatures T/T_0) are (a): 1.5×10^{10} (1.32); (b): 1.3×10^{10} (1.23); (c): 1×10^{10} (1.08); (d): 5×10^9 (0.76); (e): 3×10^9 (0.59); (f): 1×10^9 (0.34); (g): 5×10^8 (0.24); (h): 1×10^8 (0.11). The maximal value adopted by the curve (h) is about 47.2.

Figure 4 compares the grand canonical prediction for the ground state fraction $\langle n_0 \rangle / \langle N \rangle$ with the microcanonical expectation value $\overline{n_0}/N$, again for $\langle N \rangle = N = 10^6$. Whereas the grand canonical and the microcanonical temperature did agree perfectly, we now find, for temperatures close to T_0, a slight, but clearly visible difference between the ground state occupation numbers for the two ensembles. This difference is genuine, i.e., it is not an artifact caused by the asymptotic formulas: it can even be found for particle numbers of the order of a few hundred, when the required numbers of partitions can still be computed exactly.

We now turn to the central question: what remains from the grand canonical fluctuation catastrophe in a microcanoni-

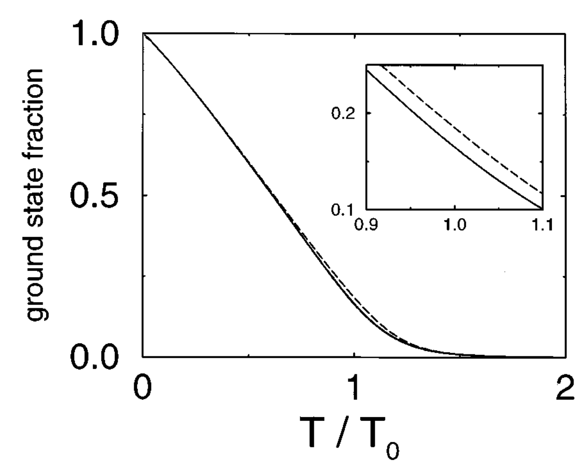

FIG. 4. Microcanonical ground state fraction $\overline{n_0}/N$ (full line) compared to its grand canonical analogue $\langle n_0 \rangle / \langle N \rangle$ (dashed), for $N = \langle N \rangle = 10^6$.

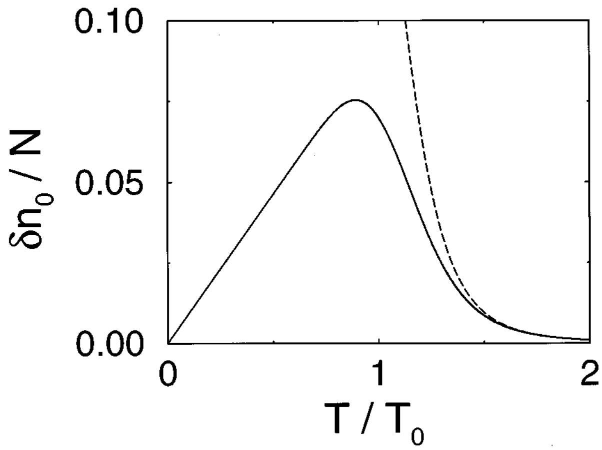

FIG. 5. Microcanonical standard deviation $\delta n_0/N$ for $N=10^6$ particles (full line); the initial slope is $\pi/(\sqrt{6}\ln N)$. The corresponding grand canonical data (dashed line) show the fluctuation catastrophe, i.e., the dramatic increase of the grand fluctuations when the ground state is occupied by a ''macroscopic'' number of particles.

cal setting? Figure 5 shows the answer. The microcanonical fluctuations $\delta n_0/N=(\overline{n_0^2}-\overline{n}_0^2)^{1/2}/N$ vanish linearly with temperature for $T\rightarrow 0$,

$$\frac{\delta n_0}{N}\approx\frac{\pi}{\sqrt{6}\ln N}\,\frac{T}{T_0}, \tag{15}$$

are maximal just below T_0, and merge into the grand canonical data above $1.5T_0$.

We remark that Fujiwara, ter Haar, and Wergeland [5] have suggested already, on the grounds of a canonical analysis, that the grand canonical expression $1+1/\langle n_0\rangle$ for the relative mean square fluctuations of the ground state population should be replaced at sufficiently low temperatures by $[(N/\overline{n}_0)-1]^2$, which vanishes properly for $T\rightarrow 0$. However, our particular microcanonical system shows a much stronger suppression of the low-temperature fluctuations: a reasonable approximation is provided by

$$\frac{(\delta n_0)^2}{\overline{n}_0^2}\approx\frac{\pi^2}{6(\ln\overline{n}_0)^2}\left(\frac{N}{\overline{n}_0}-1\right)^2. \tag{16}$$

In conclusion, we have presented a fairly complete comparison between the grand canonical and the microcanonical theory of an ideal, one-dimensional Bose gas confined by the potential of a harmonic oscillator. Whereas the grand canonical approach proceeds along standard lines, the key to the microcanonical theory is the distribution $w(n_0|m)$ introduced in Eq. (14). In view of the current interest in Bose-Einstein condensation in harmonic traps, a microcanonical derivation of its three-dimensional analogue would be most desirable. Within the grand canonical approach, Bose-Einstein condensation in three-dimensional harmonic potentials is well understood, both for very large $\langle N\rangle$ [9,18] and for the comparatively small particle numbers [19] that characterize the current experiments [1–3]. However, these experiments seem to require a microcanonical description. As in our one-dimensional system, the actual behavior of the ground state occupation number might differ measurably from the grand canonical prediction at the onset of condensation.

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