Fluctuations of the Particle Number in a Trapped Bose-Einstein Condensate

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(Received 21 May 1997)

We develop a reliable procedure for calculating the microcanonical fluctuations of the ground state occupation number for harmonically trapped ideal Bose gases, and show that these fluctuations vanish uniformly when the temperature approaches zero. The key point is the precise determination of the number of microstates from the *canonical* partition sum, thus avoiding a failure of the usual saddle point method. We also demonstrate why the magnitude of the condensate fluctuations does not depend on the total particle number. [S0031-9007(97)04478-5]

PACS numbers: 03.75.Fi, 05.30.Jp, 32.80.Pj

The ideal Bose gas, though intensely studied for decades [1,2], continues to serve as an important paradigm of quantum statistical mechanics. After the dramatic progress that has been made in the preparation and investigation of Bose-Einstein condensates of alkali atoms [3], the emphasis has been shifted from the traditional textbook example of the homogeneous gas in the thermodynamic limit [4,5] to systems consisting of large, but finite numbers of Bose particles trapped by an external potential. Such a potential drastically alters the properties of the gas: for instance, Bose-Einstein condensation occurs as a two-step process in highly anisotropic potentials [6].

One of the most demanding questions that the theory of an ideal, trapped Bose gas has to answer concerns the fluctuations δN_0 of the mean ground state occupation number N_0. Apart from their intrinsic theoretical interest, such fluctuations should play a major role in experiments with Bose-Einstein condensates at nonzero temperatures. The difficulty to calculate the precise magnitude of these fluctuations stems from the fact that this problem falls outside the scope of the conventional grand canonical treatment. Within a grand canonical setting, i.e., when the system exchanges both energy and particles with a reservoir, the mean square fluctuations of N_0 are given by $(\delta N_0)^2 = N_0(N_0 + 1)$ [4,5], implying that δN_0 becomes of order N when the temperature approaches zero. However, a Bose gas in a trap can neither exchange energy nor particles with a reservoir, so that the actual, *microcanonical* fluctuations of the ground state occupation number have to vanish with vanishing temperature.

Although this problem has been realized some time ago [7], methods for computing microcanonical bosonic ground state fluctuations begin to emerge only now [8]. A system that can be treated analytically is a gas of N Bose particles in a *one-dimensional* harmonic potential. For this model system the fluctuations of δN_0 vanish linearly with temperature T, if T is small compared to the temperature $T_0^{(1)}$ where N_0 becomes appreciable [9,10]:

$$\delta N_0 \approx \frac{\pi}{\sqrt{6}} \frac{k_B T}{\hbar\omega} \quad \text{for } T < T_0^{(1)} \equiv \frac{\hbar\omega}{k_B} \frac{N}{\ln N} . \qquad (1)$$

In a first attempt to study the fluctuations for the more realistic case of a three-dimensional ideal Bose gas trapped by an isotropic harmonic potential, Gajda and Rzążewski obtained a startling result. According to their calculation [11], the fluctuations remain comparatively high even at fairly low temperatures, which seems to require that there exists a certain temperature where the fluctuations bend sharply down in order to reach the proper zero-temperature limit. However, as we shall show in this paper, this is not the case. Although there actually exists a distinguished temperature below the condensation temperature, namely, the *restriction temperature* T_R below which the thermodynamics of the trapped Bose gas becomes exactly equivalent to that of a gas of massless excitation quanta of a system of distinguishable, i.e., Boltzmannian oscillators, the temperature dependence of the fluctuations does not change at T_R. We will develop and test a reliable procedure for calculating the microcanonical fluctuations δN_0, and show that these fluctuations approach zero in a *uniform way.*

We consider a gas of noninteracting Bosons confined in d dimensions by the potential of a harmonic oscillator; for $d > 1$ we assume the potential to be isotropic. Introducing the variable $x = \exp(-\hbar\omega/k_B T)$, where ω denotes the oscillator frequency and k_B is the Boltzmann constant, the grand canonical partition sum pertaining to this system can be written in the form

$$\mathcal{Z}^{(d)}(z,x) = \prod_{j=0}^{\infty} \frac{1}{(1 - zx^j)^{g_j}} = \sum_{N=0}^{\infty} z^N Z_N^{(d)}(x) , \qquad (2)$$

where z is the fugacity, g_j is the degree of degeneracy of the jth single-particle state [hence $g_j = 1$, $(j+1)$, or $(j+1)(j+2)/2$ for $d = 1, 2,$ or 3, respectively], and

$$Z_N^{(d)}(x) = \sum_{n=0}^{\infty} x^n \Omega^{(d)}(n|N) \qquad (3)$$

are the canonical N-particle sums. We use the symbol $\Omega^{(d)}(n|N)$ to denote the number of possibilities to distribute n excitation quanta over N particles, subject to Bose symmetry, which is the number of microstates that are accessible when the excitation energy equals $n\hbar\omega$. Hence,

$\ln[\Omega^{(d)}(n|N)]$ gives the microcanonical entropy for an N-particle Bose gas.

To determine the number of microstates $\Omega^{(d)}(n|N)$ is a difficult enterprise. However, the problem simplifies considerably when n does not exceed N: When enumerating the accessible microstates, one then does not have to consider the restriction that arises from the fact that the number of particles is finite, and can proceed as if one could distribute the n quanta over infinitely many particles. Consequently, $\Omega^{(d)}(n|N)$ does not depend on N for $n \leq N$. We will denote the number of microstates by $\Omega^{(d)}(n)$ in this case.

It is thus of interest to compute the canonical partition sum $Z_\infty^{(d)}(x)$, which will correctly describe the thermodynamics of the Bose gas for temperatures lower than the restriction temperature $T_R^{(d)}$, the latter being determined by the condition that $n = N$. In the one-dimensional case, this canonical partition sum is just the generating function pertaining to the unrestricted linear partitions of an integer n [12,13]:

$$Z_\infty^{(1)}(x) = \prod_{j=1}^{\infty} \frac{1}{1 - x^j}. \tag{4}$$

Namely, if we expand the geometric series,

$$\prod_{j=1}^{\infty} \frac{1}{1 - x^j} = \sum_{n_1=0}^{\infty} x^{n_1} \sum_{n_2=0}^{\infty} x^{2n_2} \sum_{n_3=0}^{\infty} x^{3n_3} \ldots, \tag{5}$$

we see that the coefficient of x^n in the expansion of $Z_\infty^{(1)}(x)$ equals the number of solutions to the equation

$$n = n_1 + 2n_2 + 3n_3 + \ldots \qquad (\text{all } n_j \geq 0), \tag{6}$$

which is the number of unrestricted partitions of n into positive integers [12]. Since n_j can be interpreted as the number of oscillators that are in their jth excited state, this number coincides with $\Omega^{(1)}(n)$. To find the analogous expression for $Z_\infty^{(d)}(x)$ for arbitrary d, we merely have to revert to this line of reasoning: Since each oscillator level now is g_j-fold degenerate, Eq. (6) is replaced by

$$n = \sum_{j=1}^{\infty} j \sum_{k=1}^{g_j} n_{jk} \qquad (\text{all } n_{jk} \geq 0). \tag{7}$$

The number of solutions to this equation, which is the number $\Omega^{(d)}(n)$ of microstates accessible at the energy $n\hbar\omega$, equals the coefficient of x^n in the expansion of

$$\prod_{j=1}^{\infty} \left(\sum_{n_j=0}^{\infty} x^{jn_j} \right)^{g_j} = \prod_{j=1}^{\infty} \frac{1}{(1 - x^j)^{g_j}} \equiv Z_\infty^{(d)}(x). \tag{8}$$

This is just the canonical partition sum of an infinite number of distinguishable harmonic oscillators, g_j of them having the frequency $j\omega (j \geq 1)$. Below the restriction temperature $T_R^{(d)}$, the thermodynamical properties of the trapped Bose gas therefore equal those of a "gas" of excitation quanta of this oscillator system. Normalizing $T_R^{(d)}$ with respect to the (approximate) condensation temperature $T_0^{(d)} = (\hbar\omega/k_B)[N/\zeta(d)]^{1/d}$, we have

$$\frac{T_R^{(d)}}{T_0^{(d)}} \approx \frac{\zeta(d)^{1/d}}{[d\zeta(d + 1)]^{1/(d+1)}} \frac{1}{N^{1/d(d+1)}} \tag{9}$$

for $d \geq 2$; $\zeta(z)$ denotes the Riemann zeta function. In particular, for $d = 3$ this gives $T_R^{(3)}/T_0^{(3)} \approx 0.792N^{-1/12}$ so that the restriction temperature is about 25% of the condensation temperature for a gas to 10^6 (real) particles, well within the reach of present experiments.

The oscillator system (8) has been studied already in 1951 by Nanda [13], who derived the asymptotic expression for $\Omega^{(3)}(n)$. Nanda's formula can be used to check the standard procedure for estimating $\Omega^{(3)}(n|N)$: Analytically continuing the grand canonical partition sum (2) and choosing contours γ_x and γ_z that encircle the origin of the complex x and z plane, respectively, while remaining within the unit circle, one has the identity

$$\Omega^{(d)}(n|N) = \frac{1}{(2\pi i)^2} \oint_{\gamma_z} dz \oint_{\gamma_z} dx \, \frac{Z^{(d)}(z,x)}{z^{N+1}x^{n+1}} \tag{10}$$

that can be evaluated approximately, for both $n \leq N$ and $n > N$, with the help of the saddle point method [11]. In Fig. 1 we compare the entropy of the actual Bose gas for $d = 3$ and $N = 10^4$ as obtained from the saddle point approximation (full line) to the corresponding entropy of our gas of excitation quanta (dashed), as obtained from Nanda's formula [13]. The inset highlights the regime $n/N \leq 1$, where $\Omega^{(3)}(n|N)$ is actually equal to $\Omega^{(3)}(n)$, and confirms the validity of the approximation. But the full figure reveals an even more important fact: The entropy of the excitation gas provides a fair approximation to the entropy of the Bose gas even above $T_R^{(3)}$, namely, right up to the condensation temperature, even though the number of exitation quanta per particle becomes significantly larger than unity. Expressed in a microcanonical language,

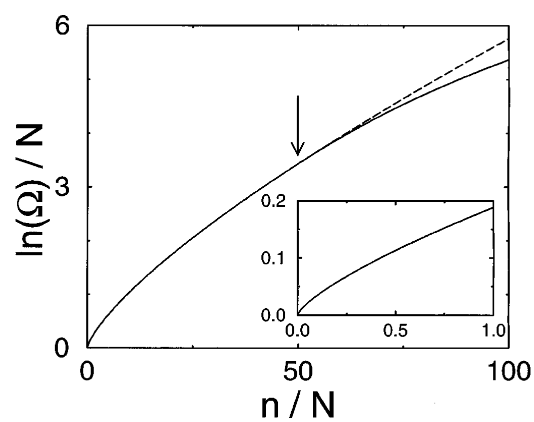

FIG. 1. Entropy of the Bose gas for $d = 3$ and $N = 10^4$ as obtained from the saddle point approximation to Eq. (10) (full line), compared to the entropy of the gas of excitation quanta described by Eq. (8) (dashed). The arrow marks the condensation point. Both entropies appear to coincide perfectly in the range $0 \leq n/N \leq 1$ (inset).

the restriction on the number of accessible microstates stemming from the fact that N is finite has only a minor effect below the condensation point.

A very accurate estimate of $\Omega^{(d)}(n|N)$ is a necessary prerequisite for determining both the ground state occupation number of an isolated Bose gas and its fluctuation [9–11]. Since $\Omega^{(d)}(n|N_{\mathrm{ex}})$ is the number of possibilities to distribute n quanta over *at most* N_{ex} particles, the difference $\Omega^{(d)}(n|N_{\mathrm{ex}}) - \Omega^{(d)}(n|N_{\mathrm{ex}} - 1)$ gives the number of microstates with n quanta distributed over *exactly* N_{ex} of the N particles, so that

$$p_{\mathrm{ex}}^{(d)}(N_{\mathrm{ex}}|n) = \frac{\Omega^{(d)}(n|N_{\mathrm{ex}}) - \Omega^{(d)}(n|N_{\mathrm{ex}} - 1)}{\Omega^{(d)}(n|N)} \qquad (11)$$

gives the probability to find N_{ex} excited particles when there are n excitation quanta present in the N-particle system. Since the remaining $N - N_{\mathrm{ex}}$ particles are in the ground state, $N - \langle N_{\mathrm{ex}}\rangle \equiv \langle N_0\rangle$ is the microcanonical expectation value for the ground state occupation number. The symbol $\langle N_{\mathrm{ex}}\rangle$ denotes, of course, the first moment of the distribution (11); its second moment yields the desired fluctuations of the ground state occupation number.

It is worthwhile to stress that the numerator on the right hand side of Eq. (11) compares $\Omega^{(d)}(n|N_{\mathrm{ex}})$ and $\Omega^{(d)}(n|N_{\mathrm{ex}} - 1)$, *not* merely their logarithms. Even though the saddle point approximation to Eq. (10) yields accurate entropies (see Fig. 1), it does not follow automatically that it also yields the numbers $\Omega^{(d)}(n|N_{\mathrm{ex}})$ themselves with an accuracy that is sufficient to determine $p_{\mathrm{ex}}^{(d)}(N_{\mathrm{ex}}|n)$. It is therefore advisable to subject the saddle point approximation to a more stringent test. Such is easily done for $d = 1$: We obviously have $\Omega^{(1)}(n|1) = 1$ and $\Omega^{(1)}(n|n) = 1$ for all n. If we then want to distribute n quanta over exactly k oscillators ($n \geq k > 1$), we first need k quanta to make sure that all of these oscillators are excited; the remaining $(n - k)$ quanta can then be distributed *ad libitum* over j of these k excited oscillators. Hence we have the recursion relation

$$\Omega^{(1)}(n|k) = \sum_{j=1}^{\min(n-k,k)} \Omega^{(1)}(n - k|j) \qquad (12)$$

that can be evaluated numerically for moderate values of n and N, so that the *exact* distribution $p_{\mathrm{ex}}^{(1)}(N_{\mathrm{ex}}|n)$ is available. The full line in Fig. 2 depicts the resulting exact fluctuations of the ground state occupation number, $\delta N_0 = (\langle N_0^2\rangle - \langle N_0\rangle^2)^{1/2}$, for $d = 1$ and $N = 1000$ versus (microcanonical) temperature, determined by $\hbar\omega T^{-1}(n) \equiv k_B \ln[\Omega^{(1)}(n|N)/\Omega^{(1)}(n - 1|N)]$. The straight line beautifully confirms the linear law (1). But the saddle point approach to Eq. (10) fails. Although this technique still yields quite good approximations to the first moments of the distributions (11), the corresponding fluctuations (long dashes) are overestimated, and do not appear to vanish properly with temperature. The reason for this failure lies in the fact that below the onset of condensation the saddle point lies very close to the first singularity of $\ln \mathcal{Z}^{(d)}(z, x)$ (see Ref. [2], p. 227), so that a condition for the applicability of the saddle point approximation is violated.

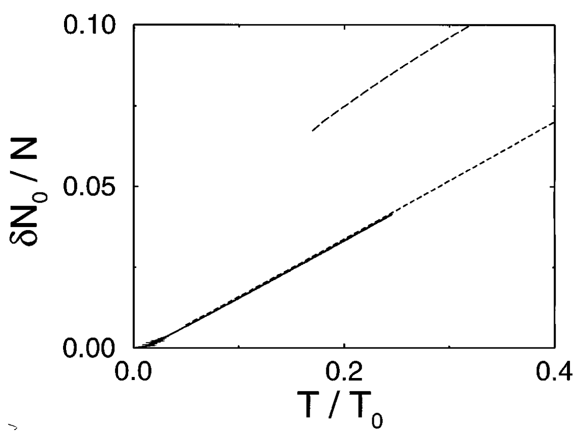

FIG. 2. Exact fluctuations $\delta N_0/N$ of the ground state occupation number for $d = 1$ and $N = 1000$ (full line), compared to the data that result from the saddle point approximation to Eq. (10) (long dashes). The short-dashed line has been obtained from the saddle point approximation to the single contour integral refers to (13).

Can one circumvent this pitfall? If one knew the *canonical* partition sums and could work within a fixed N-particle sector right from the outset, one could do away with one of the contour integrals in Eq. (10) and determine the numbers $\Omega^{(d)}(n|N)$ from the identity

$$\Omega^{(d)}(n|N) = \frac{1}{2\pi i} \oint_{\gamma_x} dx\, \frac{Z_N^{(d)}(x)}{x^{n+1}}. \qquad (13)$$

In fact, the canonical N-particle partition function *is* well known for $d = 1$ [14,15]:

$$Z_N^{(1)}(x) = \prod_{j=1}^{N} \frac{1}{1 - x^j}, \qquad (14)$$

which is nothing but the generating function for the linear partitions of an integer n into exactly N parts [12]. This allows us to calculate $\Omega^{(1)}(n|N)$ by means of the saddle point approximation to the single contour integral (13); this approximation rests on a fairly solid mathematical basis [16]. The short-dashed line in Fig. 2 shows the resulting fluctuations $\delta N_0/N$ for the example considered above: The agreement with the exact data could hardly be any better.

The attempt to extend this procedure to higher d hinges on the problem that no closed expressions are known for the partition functions $Z_N^{(d)}(x)$, which, after all, embody all the exchange correlations. However, there exists a general recursion relation that links an N-particle partition function at a certain temperature T to all k-particle partition functions with $k < N$ at the same T, and to the single-particle partition function at temperatures T/k [17–19]. Applied to the isotropic oscillator, this relation reads

$$Z_N^{(d)}(x) = \frac{1}{N} \sum_{k=1}^{N} Z_1^{(d)}(x^k) Z_{N-k}^{(d)}(x), \qquad (15)$$

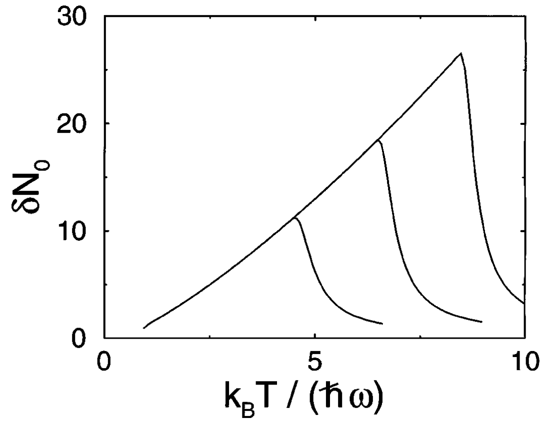

FIG. 3. Microcanonical fluctuations δN_0 for $d = 3$ and $N = 200$, 500, and 1000. The fluctuations are maximal close to the respective condensation point. Note that the low-temperature fluctuations are independent of N.

with $Z_1^{(d)}(x) = 1/(1 - x)^d$. We thus can generate the required partition functions recursively, and then compute the fluctuations within the saddle point approximation to Eq. (13), in analogy to the case $d = 1$. Figure 3 shows the result for $d = 3$ and $N = 200$, 500, and 1000. The fluctuations exhibit a sharp maximum close to the respective condensation point, and then decrease uniformly with decreasing T, without changing their behavior at the restriction temperature. For $N = 1000$, the maximal microcanonical fluctuations $\delta N_0/N$ reach about 2.7%.

Figure 3 demonstrates that the low-temperature condensate fluctuations are independent of the total particle number N. Such a behavior is obvious below the restriction temperature, since then there exist no microstates with all the particles being excited, so that all the system's properties become strictly independent of N. However, the N-independence actually persists almost up to the condensation temperature: Even if $n > N$, but $T < T_0^{(d)}$, those microstates where all the particles are excited evidently carry only negligible statistical weight. This is the reason why the fluctuations (1) are manifestly independent of N, and why the Boltzmannian oscillator system (8) can describe the thermodynamics of the trapped Bose gas up to the condensation temperature, although its partition function (8) does not depend on N.

It is now a major challenge to extend the microcanonical approach to weakly interacting Bose gases. Even though weak interactions would, in all likelihood, reduce the grand canonical fluctuation catastrophe [20], the true condensate fluctuations of weakly interacting, isolated Bosons will have to be computed microcanonically. The present work, providing the first accurate results on microcanonical, ideal condensate fluctuations in three-dimensional traps, may serve as a starting point for such a development.

We thank B. Eckhardt (Marburg), D. H. E. Groß (Berlin), and K. Kirsten (Leipzig) for valuable discussions.

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