

Trapped Bose gas: The canonical versus grand canonical statistics

C. Herzog and M. Olshanii*

Lyman Laboratory, Harvard University, Cambridge, Massachusetts 02138

(Received 15 November 1996)

For ensemble of bosons trapped in a one-dimensional harmonic potential well we have found an analytical formula for the canonical partition function and shown that, for 100 trapped atoms, the discrepancy between the grand canonical and the canonical predictions for the condensate fraction reaches 10% in the vicinity of the Bose-Einstein threshold. This discrepancy decreases only logarithmically as the number of atoms increases. Furthermore, we investigate numerically the case of a three-dimensional ‘‘cigar-shape’’ trap in the range of parameters corresponding to current Bose-Einstein condensation experiments. [S1050-2947(97)02004-0]

PACS number(s): 03.75.Fi, 05.30.Jp

Recently, Bose-Einstein condensation (BEC) in trapped atomic gases [1,2] has been realized. The trapped atomic cloud possesses two remarkable features: First, the system is small enough so that finite particle effects are potentially observable, and second, particle interactions are weak. The thermodynamics of such a system is an interesting and rich area for scientific analysis.

The equivalence of the grand canonical and fixed- N canonical descriptions of a statistical system is an old question widely discussed in the textbooks on statistical mechanics [3,4]. For a bosonic gas, where grand canonical fluctuations of the ground-state population become large at and below the Bose-Einstein threshold, such an equivalence is not obvious. It is shown that in the thermodynamic limit $N \rightarrow \infty$ both ensembles give the same predictions for the mean values of occupation numbers even in the absence of particle interactions [5]. Furthermore, it is well known that for large N , interactions between particles lead to suppression of fluctuations in the grand canonical ensemble [4]. However, for a finite system with a mesoscopic number of particles, the equivalence of the two ensembles is not ensured.

The main scaling laws for the fluctuations in an ideal canonical bose gas were derived by Fujiwara *et al.* [5]. The fixed- N Bose statistics is shown to be closely related to Gentile’s grand canonical intermediate statistics [6]. Krauth performed fixed- N finite temperature Monte Carlo calculations for a three-dimensional (3D) harmonic potential [7]. Although the main subject of the paper [7] is the role of interactions, it is shown also that, for macroscopic numbers of particles, the noninteracting grand canonical and canonical ensembles agree very well. These conclusions are consistent with the numerical results of Politzer [8]. In the present paper we consider *mesoscopic* values of number of particles ($N \sim 100$) confined in a one-dimensional harmonic trap [9] and in a three-dimensional ‘‘cigar-shape’’ trap. We show that the difference between using grand canonical and canonical statistics is *substantial*.

Consider an ensemble of N noninteracting bosons confined in a 1D harmonic potential in thermal (but not in diffusive) equilibrium with a large reservoir. The population

distribution among the different energy levels of the N -particle system will be given by the Boltzmann law

$$\rho([n]) \sim \exp\{-\beta E([n])\}, \quad (1)$$

$$[n] = \left\{ n_0, n_1, \dots, n_s, \dots \left| \sum_s n_s = N \right. \right\}, \quad (2)$$

where $E([n]) = \sum_s n_s \epsilon_s$ is the N -particle energy for the given configuration of occupation numbers $[n]$, $\epsilon_s = \hbar \omega s$ ($s = 0, 1, 2, \dots$) is the single particle energy spectrum, ω is the harmonic-oscillator frequency, $\beta = 1/k_B T$, and T is the temperature of the system. Note that, in the harmonic-oscillator case, the N -particle energy is quantized as

$$E([n]) = \hbar \omega K, \quad (3)$$

where $K = \sum_s n_s s$.

To calculate mean occupation numbers of the oscillator states, we need to know the partition function Q and its derivatives. We show below that in the 1D harmonic oscillator case, occupation numbers may be calculated analytically as finite sums of finite products. The canonical partition function $Q(\beta, N)$ can be represented by a power series of $x = \exp(-\beta \hbar \omega)$:

$$Q(\beta, N) = \sum_{K=0}^{\infty} x^K \Gamma(K, N). \quad (4)$$

The microcanonical partition function

$$\Gamma(K, N) = \sum_{\substack{[n] \\ \sum_s n_s = N, \sum_s n_s s = K}} 1 = \sum_{N'=0}^N \sum_{\substack{[n]' \\ \sum'_s n'_s = N', \sum'_s n'_s s = K}} 1 \quad (5)$$

equals the number of representations (partitions) of K as an unordered sum of at most N positive integers. Here N' is the total population of the excited states, $[n]' = \{n'_1, n'_2, \dots, n'_s, \dots\}$ is a particular configuration of excited state occupation numbers, and the ‘‘primed’’ sum $\sum' = \sum_{s=1}^{\infty}$ denotes a sum over the excited states.

According to a well-known number theory theorem [10] *the number $\Gamma(K, N)$ of partitions of K with at most N*

*Electronic address: maxim@atomsun.harvard.edu

parts equals the number $\mathcal{P}(K,N)$ of partitions of K with parts not exceeding N . Hence the canonical partition function (4) is nothing else but the generating function for the restricted partition function $\mathcal{P}(K,N)$ [10]:

$$\begin{aligned} Q(\beta,N) &= \sum_{K=0}^{\infty} x^K \mathcal{P}(K,N) \\ &= \prod_{q=1}^N \frac{1}{1-x^q}. \end{aligned} \quad (6)$$

Derivatives of the partition function $Q_s = -\beta^{-1}(\partial Q/\partial \epsilon_s)$ cannot be found directly from expression (6), which is specific for the 1D harmonic oscillator. Instead, we have found a *general* recursion relation between the canonical partition function and its derivatives:

$$Q_s(\beta,N+1) = \exp(-\beta \epsilon_s) [Q_s(\beta,N) + Q(\beta,N)]. \quad (7)$$

This relation can be applied to any fixed- N , noninteracting, bosonic system.

Finally, the mean occupation numbers are given by

$$\langle n_s \rangle = \frac{Q_s}{Q} = \sum_{q=1}^N x^{(N-q+1)s} \prod_{q=q}^N (1-x^q). \quad (8)$$

This expression is easy to analyze in the continuous limit with respect to N . For example, below the BEC threshold, the condensate population is approximately given by

$$\begin{aligned} \frac{\langle n_0 \rangle}{N} &\approx 1 - \frac{k_B T}{N \hbar \omega} (\ln(k_B T / \hbar \omega) + C + o(1)) \\ &\xrightarrow{N \rightarrow \infty} 1 - \frac{T}{T_c}, \end{aligned} \quad (9)$$

where $C \approx 0.5772$ is the Euler constant. The transition temperature is given by

$$N = \frac{k_B T_c}{\hbar \omega} \ln \left(\frac{\text{const} \times k_B T_c}{\hbar \omega} \right), \quad (10)$$

where the choice of const is a matter of convention. Note that the thermodynamic limit (9) coincides with the one predicted for grand canonical statistics [9].

Now we are ready to compare the canonical and grand canonical predictions for the condensate population $\langle n_0 \rangle$. In Fig. 1 we plot the population of the ground state for different numbers of particles. For the grand canonical predictions we simply repeat the finite-system calculations of [9]. To facilitate the comparison, we made the same choice const=2 in expression (10). Both curves approach the thermodynamic limit (9) as the number of particles increases. However, for a finite number of particles the discrepancy between the two models is quite significant. In the vicinity of the BEC threshold, the relative deviation $(\langle n_0^{\text{gr. canon.}} \rangle - \langle n_0^{\text{canon.}} \rangle) / \langle n_0^{\text{canon.}} \rangle$ decreases slowly with N and goes from 10% for 100 atoms to 5% for 10 000 atoms. We have checked that this deviation decreases according to a $1/\ln(N)$ scaling law for a fixed T/T_c . Note that the rate at which both the grand canonical

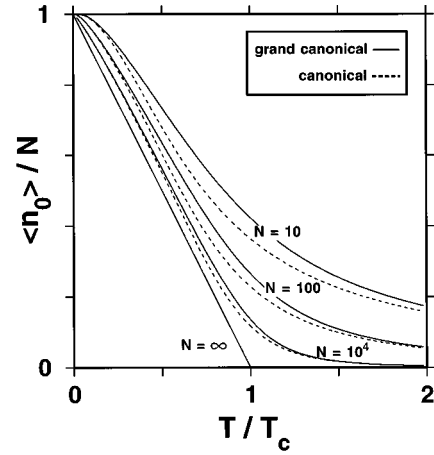


FIG. 1. The condensate fraction for the 1D harmonic oscillator as a function of temperature. Both grand canonical and canonical predictions are shown. The straight line is the thermodynamic limit (9).

[9] and canonical [Eq. (9)] populations approach the thermodynamic limit also obeys this law.

We turn now to the 3D trap. To our knowledge there is no simple analytic expression for the canonical partition function in this case. Numerically, it can be calculated by integration of the grand canonical partition function in the complex plain of chemical potential [5,8]. Indeed

$$\begin{aligned} Q(\beta,N) &= \sum_{\substack{[n] \\ \sum n_s = N}} \exp\{-\beta E([n])\} \\ &= \sum_{[n]} \delta_{\sum n_s, N} \exp\{-\beta E([n])\} \\ &= \frac{\beta}{2\pi i} \int_{-\pi i}^{+\pi i} d\mu \exp(-N\mu) Z(\beta, \mu), \end{aligned} \quad (11)$$

where

$$Z(\beta, \mu) = \prod_{s_x, s_y, s_z=0}^{\infty} \frac{1}{1 - \exp\left[-\beta \left(\sum_{\alpha=x,y,z} \hbar \omega_{\alpha} s_{\alpha} - \mu \right)\right]} \quad (12)$$

is the grand canonical partition function, ω_{α} ($\alpha=x,y,z$) are the trap frequencies, and the expression $\delta_{q,q'} = (2\pi i)^{-1} \int_{-\pi i}^{+\pi i} d\xi \exp[(q-q')\xi]$ for the Kronecker delta has been used. Derivatives of the partition function can be expressed through $Z(\beta, \mu)$ in the same way.

In Fig. 2 we plot the condensate fraction as a function of temperature for both grand canonical and canonical ensembles. We have chosen the ‘‘cigar-shape’’ configuration $\omega_{\perp} = 17.78\omega_z$, where $\omega_{\perp} = \omega_x = \omega_y$. The three-dimensional Bose-Einstein transition temperature is given by

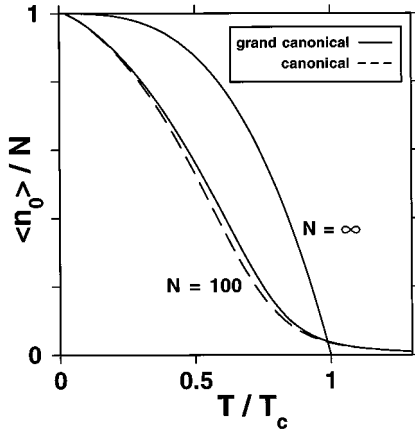


FIG. 2. The condensate fraction for a 3D “cigar-shape” trap as a function of temperature. Both grand canonical and canonical predictions are shown. Here $\omega_{\perp} = 2\pi \times 101$ Hz, $\omega_z = 2\pi \times 5.7$ Hz, $N = 100$, and $T_c = 6.5$ nK. The thermodynamic limit $N = \infty$, Eq. (14) is also shown.

$$N = g_3(1) \frac{(k_B T_c)^3}{\hbar^3 \prod_{\alpha=x,y,z} \omega_{\alpha}} + \frac{g_2(1)}{2} \frac{(k_B T_c)^2 \sum_{\alpha=x,y,z} \omega_{\alpha}}{\hbar^3 \prod_{\alpha=x,y,z} \omega_{\alpha}} + \mathcal{O}(k_B T_c / \hbar \omega), \quad (13)$$

where the second line is the finite- N correction [9]. Here $g_d(z) = \sum_{j=1}^{\infty} z^j / j^d$ is the Bose-Einstein function. For comparison, we have also plotted the thermodynamic limit

$$\frac{\langle n_0 \rangle}{N} = 1 - \left(\frac{T}{T_c} \right)^3. \quad (14)$$

For 100 particles, depending on the temperature, the system exhibits both 3D and 1D characteristics. At $T \sim 0.4 T_c$ the temperature reaches the zero-point energy $\hbar \omega_{\perp} / 2$ for transverse oscillations. The discrepancy between the grand canonical and canonical predictions is less than in the purely 1D system but is still close to 10%.

In the above discussion we neglected particle interactions. To estimate the importance of interactions in our model, we consider the “worst” case of zero temperature where the spatial density is the highest and therefore the interactions are strongest. For typical Ioffe-Pritchard trap parameters [11] ($\omega_{\perp} = 2\pi \times 101$ Hz, $\omega_z = 2\pi \times 5.7$ Hz, $N = 100$) for sodium atoms (scattering length $a = 92$ bohr, atomic mass $M = 23$ amu) the mean-field corrections to the oscillation frequencies are quite small: $\delta \omega_{\perp} = 0.03 \omega_{\perp}$ and $\delta \omega_z = 0.15 \omega_z$. To estimate the corrections, we minimized the Gross-Pitaevskii energy functional with a ground-state oscillator wave function seeded with unknown frequencies [12]. Note that for the parameters chosen, the system exhibits a BEC transition at $T_c = 6.5$ nK.

We acknowledge fruitful discussions with H. D. Politzer, T. H. Bergeman, J. H. Thywissen, E. Heller, L. You, M. Prentiss, and W. Ketterle. M.O. was supported by the National Science Foundation grant for light force dynamics No. PHY-93-12572. C.H. was supported by Harvard University. This work was partially supported by the NSF through a grant for the Institute for Theoretical Atomic and Molecular Physics at Harvard University and the Smithsonian Astrophysical Observatory.

- [1] M. H. Anderson *et al.*, *Science* **269**, 198 (1995).
- [2] K. B. Davis *et al.*, *Phys. Rev. Lett.* **75**, 3969 (1995).
- [3] C. Kittel and H. Kroemer, *Thermal Physics*, 2nd ed. (Freeman, San Francisco, 1980).
- [4] K. Huang, *Statistical Mechanics*, 2nd ed. (Wiley, New York, 1987).
- [5] I. Fujiwara *et al.*, *J. Stat. Phys.* **2**, 329 (1970).
- [6] G. Gentile, *Nuovo Cimento* **17**, 493 (1940).
- [7] W. Krauth, *Phys. Rev. Lett.* **77**, 3695 (1996).

- [8] H. D. Politzer, *Phys. Rev. A* **54**, 5048 (1996).
- [9] W. J. Mullin (unpublished); W. Ketterle and N. J. van Druten, *Phys. Rev. A* **54**, 656 (1996).
- [10] L. E. Dickson, *Diophantine Analysis*, History of the Theory of Numbers Vol. II (Chelsea, New York, 1952).
- [11] T. Bergeman *et al.*, *Phys. Rev. A* **35**, 1535 (1987); D.E. Pritchard, *Phys. Rev. Lett.* **51**, 1336 (1983).
- [12] G. Baym and C. J. Pethick, *Phys. Rev. Lett.* **76**, 6 (1996).