# Number fluctuation and the fundamental theorem of arithmetic

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We consider $N$ bosons occupying a discrete set of single-particle quantum states in an isolated trap. Usually, for a given excitation energy, there are many combinations of exciting different number of particles from the ground state, resulting in a fluctuation of the ground state population. As a counterexample, we take the quantum spectrum to be logarithms of the prime number sequence, and using the fundamental theorem of arithmetic, find that the ground state fluctuation vanishes exactly for *all* excitations. The use of the canonical or grand canonical ensembles, on the other hand, gives a substantial number fluctuation for the ground state. This is an example of a system where canonical and grand canonical ensemble averagings are not valid because of the peculiar nature of the quantum spectrum.

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After the experimental discovery of Bose-Einstein condensate in a trapped dilute gas at ultralow temperatures, much attention has been paid to the problem of number fluctuation in the ground state of the ideal system [1–9], as well as a weakly interacting Bose gas [10–17]. There are also a few papers on ground state fluctuations in a trapped Fermi gas [18]. There are several reasons for this interest. In standard statistical mechanics, number fluctuation is related to density-density correlation, and to the compressibility of the system in the grand canonical ensemble [17]. The cross section for light scattering off the medium, in principle, may be related to the ground state fluctuation in the system [19]. The so called grand canonical catastrophe in an ideal Bose gas, where the fluctuation diverges at low temperatures, was already known [20]. Therefore, a more accurate treatment of the problem was needed for trapped gases. In the microcanonical treatment of number fluctuation from the ground state in a harmonic trap, the problem is closely related to the combinatorics of partitioning an integer, and thus there was an interesting link to number theory [1]. It turned out that the result for the ground state number fluctuation was very sensitive to the asymptotic approximations that were made. Another aspect that drew much attention in the literature was the difference in the calculated results for fluctuation using the canonical and the microcanonical formulations [7,8].

In this paper, we give an example of a quantum spectrum that has no number fluctuation in the ground state for any excitation energy in the microcanonical ensemble, as a direct corollary of the fundamental theorem of arithmetic. The canonical ensemble, on the other hand, yields a dramatically different ground state number fluctuation. This failure signals the breakdown of the canonical ensemble itself due to the peculiar nature of the single-particle spectrum in our example. Generally, when a large excitation energy is supplied to a system, there is a very large number of distinct microscopic configurations accessible to it. All these different microstates describe the same macrostate of a given excitation energy. The classic example is that of bosons in a harmonic trap, where the number of partitions of an integer number, corresponding to the number of microstates, increases exponentially. We use, on the other hand, another example from number theory, to propose a system where *the excitation energy, no matter how large, is locked in one microstate*. Consequently, although it is possible to explicitly calculate the canonical or grand canonical partition functions and therefore the thermodynamic entropy for this example, it does not approach or equal the information-theoretic entropy that can be exactly calculated using number theory [22]. So far as we know, this constitutes an important example of a quantum spectrum where the usual statistical concepts fail, no matter how large the number of particles.

We consider bosons in a hypothetical trap with a single-particle spectrum (*not* including the ground state, which is at zero energy),

$$\epsilon_p = \ln p, \tag{1}$$

where $p$ runs over the prime numbers 2,3,5, . . . . We do not know how to realize such a spectrum experimentally, and it is merely a means of performing a thought experiment. We shall use, in what follows, both a truncated sequence of primes as well as the infinite sequence when we perform the canonical calculations for fluctuation. First, however, we perform the exact calculation for number fluctuation from the ground state. Suppose that there are $N$ bosons in the ground state at zero energy, and an excitation energy $E_x$ is given to the system. In how many ways can this energy be shared amongst the bosons by this spectrum? Before giving the answer, we remind the reader of the fundamental theorem of arithmetic, which states that every positive integer $n$ can be written in only one way as a product of prime numbers [23]:

$$n = p_1^{n_1} p_2^{n_2} \cdots p_r^{n_r} \cdots, \tag{2}$$

where $p_r$'s are distinct prime numbers, and $n_r$'s are positive integers including zero, and need not be distinct. It immediately follows from Eq. (2) that if the excitation energy $E_x = \ln n$, where the integer $n \geqslant 2$, there is only one unique way of exciting the particles from the ground state. If $E_x \neq \ln n$, the energy is not absorbed by the quantum system. Since the number of bosons excited from the ground state, for a given $E_x$, is unique for this system, *the number fluctuation in the ground state is identically zero*. Moreover, this conclusion is valid whether we take in Eq. (1) an upper cutoff in the prime number, or the infinite sequence of all the primes. The information-theoretic entropy at an excitation energy $E_x$ is

$$\mathcal{S}(E_x) = -\sum_i P_i \ln P_i , \tag{3}$$

where $P_i$ is the probability of excitation of the microstate $i$. Since only one microstate contributes with unit probability, and all others have $P_i=0$ (when $E_x=\ln n$), the entropy $\mathcal{S}=0$. It is also straightforward to calculate the ground state population $N_0$ as a function of the excitation energy $E_x$. For this purpose, we truncate the spectrum given by Eq. (1) to the first $10^6$ primes, with a cutoff denoted by $p^\star$, and take $N=100$. We shall display the numerical results after describing the canonical calculations.

Our next task is to calculate these quantities in the canonical ensemble, and see if the differences in the microcanonical and canonical results may be accounted for (as $N\to\infty$) using the method of Navez *et al.* [7]. We first do the calculation for the truncated spectrum. The one-body canonical partition function is then given by $Z_1(\beta)=1+\sum_{p=2}^{p^\star}\exp(-\beta\ln p)$. The $N$-body bosonic canonical partition function is obtained by using the recursion relation [24]

$$Z_N(\beta) = \frac{1}{N}\sum_{s=1}^{N} Z_1(s\beta) Z_{N-s}(\beta). \tag{4}$$

Once $Z_N$ is found, the ground state occupation $N_0=\langle n_0\rangle_N$ and the ground state number fluctuation for the canonical ensemble can be readily computed [18,25]. We define $\langle\delta^2 N_0\rangle=(\langle n_0^2\rangle_N-\langle n_0\rangle_N^2)$, where the right-hand side (RHS) is calculated using Eqs. (24) and (25) of Ref. [18]. In Figs. 1(a) and 1(b), we display the results of the canonical calculations for the ground state occupancy fraction $N_0/N$ and the ground state fluctuation $\langle\delta^2 N_0\rangle^{1/2}/N$ for $N=100$ as a function of temperature $T$ with the truncated spectrum of the first $10^6$ primes. For comparison, we also show the results of the corresponding grand canonical calculation. The grand canonical catastrophe for the number fluctuation is clearly evident. It is also easy to calculate the canonical (equilibrium) entropy $S=\ln Z_N(\beta)+\beta\langle E_x\rangle$, where the average excitation energy is given by $\langle E_x\rangle=-\partial\ln Z_N(\beta)/\partial\beta$. The comparison with the combinatorial (or microcanonical) results requires that we identify the excitation energy $E_x$ with the canonical average $\langle E_x\rangle$. This is only true if $\langle E_x\rangle$ is sharply peaked at the equilibrium temperature, as a consequence of the competition between the increasing number of accessible states with temperature, and the decrease in the corresponding occupancy due to the Boltzmann weighting. In the particular example under study, the canonical concept of averaging breaks down. This is apparent in Fig. 2, where the canonical fractional occupancy of the bosons in the excited states, $\langle N_e\rangle/N$, for $N=100$, is compared with the (exact) combinatorial (or microcanonical) calculation as a function of the excitation energy $E_x$. Although the canonical and the grand canonical $\langle N_e\rangle/N$ are nearly identical, the corresponding microcanonical quantity is radically different. This anomaly persists even as $N\to\infty$, showing the breakdown of the equivalence between the microcanonical and the other ensembles. In Fig. 3, we display the behavior of the canonical entropy as a function of $T$ and $\langle E_x\rangle$. The microcanonical entropy $\mathcal{S}(E_x)$, of course, is zero, and so is the number fluctuation $\langle\delta^2 N_0\rangle$. Thus, we find that the canonical results have no resemblance with the exact microcanonical ones. All these calculations were performed for a truncated spectrum (first $10^6$ primes) of $\ln p$, as specified earlier, and for $N=100$.

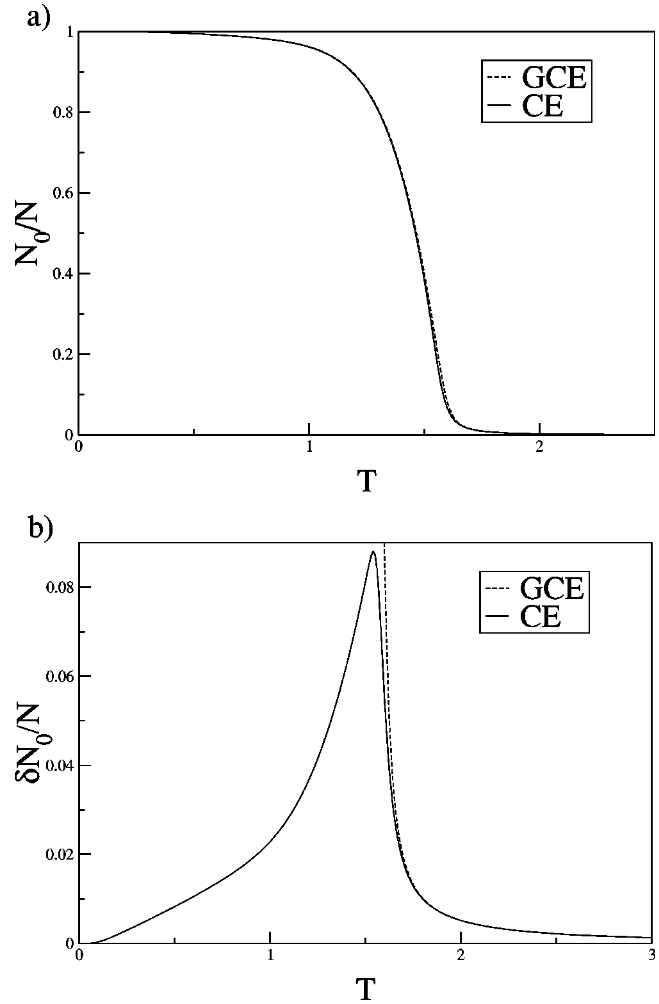


FIG. 1. (a) Average occupancy in the ground state, $N_0/N$, versus temperature $T$ for $N=100$ in the canonical and grand canonical ensembles. (b) Plot of the relative ground state number fluctuation in both ensembles. Note the steep rise in the grand canonical fluctuation.

It was pointed out by Navez *et al.* [7] that for a trapped Bose gas below the critical temperature, the microcanonical result for fluctuation could be obtained solely using the canonically calculated quantities, which in turn may be obtained from the so called Maxwell-Demon ensemble [21]. We now use this procedure to check if the microcanonical results may be obtained from a canonical calculation as $N\to\infty$. These authors constructed the Maxwell-Demon ensemble in which the ground state (for $T<T_c$) was taken to be the reservoir of bosons that could exchange particles with the rest of the subsystem (of the excited spectrum) without exchanging energy. Denoting the grand canonical partition

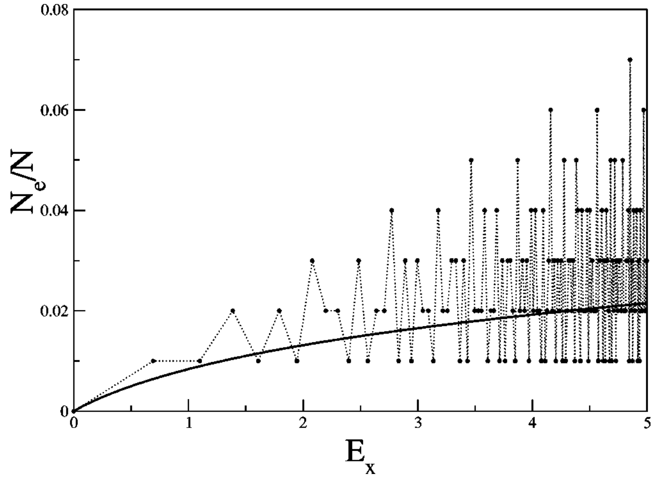


FIG. 2. Plot of the average occupancy in the excited states, $N_e/N$, for $N=100$, versus the excitation energy $E_x$ in the canonical ensemble (continuous bold curve), compared with the exact microcanonical calculation. As emphasized in the text, for the canonical calculation, the ensemble averaged $\langle E_x \rangle$ is identified with the excitation energy $E_x$. The microcanonical calculation is done for $E_x = \ln n$, where $n$ is an integer, and the results are shown by dark points. These are joined by dotted lines to emphasize their zigzag character. For example, the sixth point (including 0) corresponds to $E_x = \ln 6$, and gives $N_e = 2$, corresponding to the prime factor decomposition $2\times 3$.

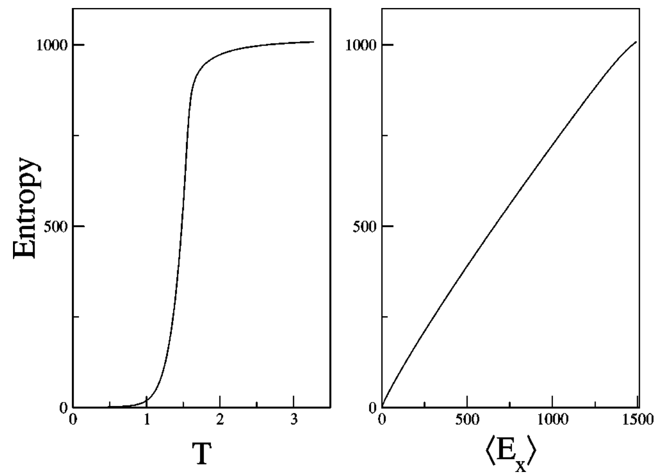


FIG. 3. Plot of the canonical entropy as a function of temperature $T$ on the left, and excitation energy $\langle E_x \rangle$ on the right, for $N=100$. The microcanonical entropy is zero.

function of the excited subsystem by $\Xi_e(\alpha,\beta)$, with $\alpha = \beta\mu$, it was shown that the canonical occupancy of the excited states, $\langle N_e \rangle$, and the number fluctuation $\langle \delta^2 N_e \rangle$ could be obtained from the first and the second derivative of $\Xi_e$ with respect to $\alpha$, and then putting $\alpha = 0$. It was further noted that the microcanonical number fluctuation for the excited particles was related to the canonical quantities by the relation

$$\langle \delta^2 N_e \rangle_{MC}^{\infty} = \langle \delta^2 N_e \rangle_{CN}^{\infty} - \frac{[\langle \delta N_e \delta E \rangle_{CN}^{\infty}]^2}{\langle \delta^2 E \rangle_{CN}^{\infty}}, \tag{5}$$

where the superscript $\infty$ denotes $N \to \infty$. This worked efficiently for harmonic traps in various dimensions. These calculations, for our system, are also easily done for $\beta > 1$. We now consider spectrum (1) to be the infinite sequence of the primes, and evaluate the RHS of Eq. (6). We readily obtain the convergent expression (for $\beta > 1$)

$$\langle \delta^2 N_e \rangle_{MC}^{\infty} = \sum_p \frac{p^\beta}{(p^\beta - 1)^2} - \frac{\left[ \sum_p \frac{(\ln p) p^\beta}{(p^\beta - 1)^2} \right]^2}{\sum_p \frac{(\ln p)^2 p^\beta}{(p^\beta - 1)^2}}. \tag{6}$$

The RHS of Eq. (6) is nonzero, and therefore does not agree with the microcanonical result. The failure of the above formalism of Navez *et al.* [7] is not a shortcoming of their method, but is due to the failure of the canonical ensemble averaging itself when applied to the single-particle spectrum (1). This is further elaborated below.

Consider constructing the $N$-particle canonical partition function $Z_N(\beta)$ from spectrum (1), as we have done. As $N \to \infty$, a little thought will show that $Z_N \to \zeta(\beta)$, where $\zeta(\beta) = \sum_n 1/n^\beta$ is the Riemann zeta function. This is because we are allowed to span over all $E$ in calculating $Z_N(\beta)$. Similarly, the grand partition function $\Xi_e(\alpha,\beta)$ with $\alpha = 0$ is none other than the Euler product representation of the Riemann zeta function [23]. This has a density of states growing exponentially with $E$, and has been studied in connection with the limiting hadronic temperature [26]. In contrast, the number of accessible states for an excitation energy $E$ in the microcanonical setup does not increase at all. Since the energy remains locked in one microstate, the system cannot be described through the usual concepts of statistical mechanics. Although the thought experiment investigated in this paper is too idealized to be realizable in the real world, it does serve as a warning that the canonical (grand canonical) ensemble averaging may yield nonsensical results if there is not a large number of microstates corresponding to a macrostate.

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