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 counter example, 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 standard canonical or grand canonical ensembles, on the other hand, gives substantial number fluctuation for the ground state. This difference between the microcanonical and canonical results cannot be accounted for within the framework of equilibrium statistical mechanics.

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After the experimental discovery of BEC in a trapped dilute gas at ultra-low temperatures, much attention has been paid to the problem of number fluctuation in the ground state of the ideal system, as well as a weakly interacting Bose gas, as a direct corollary of the fundamental theorem of arithmetic. This failure of the canonical (grand canonical) ensembles is 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 are a very large number of distinct microscopic configurations that are accessible to it. All these different microstates describe the same macro-state of a given excitation energy. The classic example is that of bosons in a harmonic trap, where the fluctuation diverges at low temperatures, was already known. Therefore a more accurate treatment of the problem was needed for trapped gases. In the microcanonical treatment of number fluctuation from the ground state, the problem is closely related to the combinatorics of partitioning an integer, and thus there was an interesting link to number theory. It turned out that the result for the ground state number fluctuation was very sensitive to the kind of asymptotic approximations that are 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. It was pointed out by Navez et al. 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, to be explained later.

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. The method of Navez et al. fails to account for the difference between the microcanonical and canonical results in this example. This failure of the canonical (grand canonical) ensembles is 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 are a very large number of distinct microscopic configurations that are accessible to it. All these different microstates describe the same macro-state 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 theoretical entropy that can be exactly calculated using number theory.

So far as we know, this constitutes a novel and new example that links number theory and thermodynamics, and gives radically different results for the microcanonical and canonical ensembles.

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

$$\epsilon_p = \ln p,$$

where $p$ runs over the prime numbers $2, 3, 5, \ldots$. Of course, such a spectrum is not realizable 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:

\[ n = p_1^{n_1} p_2^{n_2} \ldots p_r^{n_r}, \]

where $p_i$’s are distinct prime numbers, and $n_i$’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 $n \geq 2$, 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. (3) an upper cut-off in the prime number, or the infinite sequence of all the primes. The information-theoretic entropy at an excitation energy $E_x$ is

\[ S(E_x) = - \sum_i P_i \ln P_i, \]

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 $S = 0$. 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. (4) to the first million primes, with a cutoff denoted by $p^*$, 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. [4]. We first do the calculation for the truncated spectrum. The one-body canonical partition function is then given by

\[ Z_N(\beta) = \frac{1}{N} \sum_{s=1}^{N} Z_1(s\beta)Z_{N-s}(\beta). \]

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 be computed [18, 25]. We define $\delta N_0^2 = (\langle n_0^2 \rangle_N - (\langle n_0 \rangle_N)^2)$, where the RHS is calculated using Eqs. (24) and (25) of Ref. [15]. In Fig. 1a) and b), we display the results of the canonical calculations for the ground state occupancy fraction $N_0/N$ and the ground state fluctuation $(\Delta N_0^2)^{1/2}/N$ for $N = 100$ as a function of temperature $T$ with the truncated spectrum of the first million 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 $S = \ln Z_N(\beta) + \beta E_x$. The comparison with the combinatorial (or microcanonical) results requires that we convert the canonical temperature to excitation energy $E_x$. This is done by using the standard relation $E_x = -\frac{\partial \ln Z}{\partial \beta}$. In Fig. 2, the canonical fractional occupancy of the bosons in the excited states, $\langle N_x \rangle /N$, 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 grandcanonical $\langle N_x \rangle /N$ 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 behaviour of the canonical entropy as a function of $T$ and $E_x$. The microcanonical entropy $S(E_x)$, of course, is zero, and so is the number fluctuation $\Delta N_0^2$. 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 million primes) of $\ln p$, as specified earlier, and for $N = 100$.

We shall now use the procedure of Navez et al. [4] to check if the microcanonical results may be obtained from a canonical calculation as $N \to \infty$. These authors constructed the so-called Maxwell’s 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 states) without exchanging energy. Denoting the grand canonical partition 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

\[ \langle \Delta^2 N_e \rangle_{MC} = \langle \Delta^2 N_e \rangle_{CN} \frac{\langle \Delta N_e \Delta E \rangle_{CN}^2}{\langle \Delta^2 E \rangle_{CN}^2}, \]
where the superscript $\infty$ denotes $N \rightarrow \infty$. This worked beautifully for harmonic traps in various dimensions. These calculations, for our system, are also easily done for $\beta > 1$. We now consider the spectrum \(3\) to be the infinite sequence of the primes, and evaluate the RHS of Eq. \(4\). We readily obtain the convergent expression (for $\beta > 1$)

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

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 because of the very special nature of the single-particle spectrum \(4\). Consider constructing the $N$-particle canonical partition function $Z_N(\beta)$ from this spectrum, as we had done. As $N \rightarrow \infty$, a little thought will show that $Z_N \rightarrow \zeta(\beta)$, where $\zeta(\beta) = \sum_n \frac{1}{n^\beta}$ 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 $\Xi(\alpha, \beta)$ 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 \(26\). By contrast, the number of accessible states with a fixed $N$ and $E$ in the isolated microcanonical set-up does not increase at all. Since the energy remains locked in one microstate, the isolated system cannot be described through the usual concepts of statistical mechanics.

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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.

FIG. 2: a) Plot of the average occupancy in the excited states $N_{ex}/N$, for $N = 100$, versus the excitation energy $E_x$ in the canonical ensemble (continuous bold curve), compared with the exact microcanonical calculation. The latter 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 $E_x$ on the right, for $N = 100$. The microcanonical entropy is zero.

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