Ground state fluctuations in finite Fermi and Bose systems

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Abstract

We consider a small and fixed number of fermions (bosons) in a trap. The ground state of the system is defined at $T = 0$. For a given excitation energy, there are several ways of exciting the particles from this ground state. We formulate a method for calculating the number fluctuation in the ground state using microcanonical counting, and implement it for small systems of noninteracting fermions as well as bosons in harmonic confinement. This exact calculation for fluctuation, when compared with canonical ensemble averaging, gives considerably different results, specially for fermions. This difference is expected to persist at low excitation even when the fermion number in the trap is large.

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I. INTRODUCTION

The traditional approach to determining the number fluctuations in a given quantum state relies on the statistical description of the system based on the grand canonical ensemble (GCE). For bosons, if $< N_i >$ is the average occupancy of a single orbital $i$, then the mean-square fluctuation in GCE is given by $< (\Delta N_i)^2 > = < N_i > (1+ < N_i >)$. As the temperature $T \to 0$ for the boson system, however, there is macroscopic occupancy in the ground state, with the result that the relative fluctuation $< (\Delta N_0)^2 >^{1/2} / N \to 1$. This is clearly absurd, since at $T = 0$, none of the bosons (in the noninteracting case) should be in the excited orbitals, so the fluctuation should vanish. This problem, first discussed by Fujiwara et al. [2], is of topical interest with the discovery of Bose-Einstein condensation in a dilute gas of alkali atoms confined in a trap [3]. The problem of number fluctuation from the ground state of a system of confined fermions is also of interest due to the recent developments in the field of quantum dots [4]. The fluctuation in Bose-Einstein systems has been addressed in a series of papers [5–9] both in micro-canonical and canonical ensemble framework. A clear and unambiguous definition of the fluctuation has been given for calculating the ground state occupation number fluctuation by Grossman and Holthaus [6] through the ”microcanonical entropy” of an N-particle Bose system. Detailed comparisons between the two methods for noninteracting bosons in a harmonic trap have been made by Holthaus and Kalinowski [7], where analytical expressions for the two are also given using a modified saddle-point approximation.

Our focus in this paper is on the exact calculation of the ground state fluctuation for a small number of fermions confined in a trap. For comparison, the corresponding calculations are also done for bosons. To this end, a combinatorial method based on microcanonical counting is developed in sect.(II), and calculations are made for particles in one and two-dimensional harmonic traps. These exact results are then compared with the corresponding canonical ensemble calculations. The two methods yield substantially different, though qualitatively similar results. As explained later, we expect this deficiency of the canonical ensemble averaging method to persist for fermions at low excitation, even when the fermion number in the trap is large. In sect.(III) we show that even though the canonical entropies for noninteracting bosons and fermions in a one-dimensional harmonic trap are identical, the number fluctuations in the ground state are vastly different. The numerical results are discussed in sect.(IV).

II. FLUCTUATIONS IN THE INDEPENDENT PARTICLE MODEL

We assume an independent particle model where the one particle partition function is given analytically, or may be computed. We first give the well-known recipe of calculating the $N$- particle quantum canonical partition system from this. At zero temperature all the particles are in the ground state. At a finite temperature, however, the excitation energy may be shared in many different ways amongst the particles, with the result that the population in the original ground state is not fixed, although the total number, $N$, is still the same. Our objective here is to define and calculate this fluctuation in the ground state occupation as a function of excitation energy or, equivalently, temperature.
The canonical partition function for bosons and fermions in any space dimension may be written as
\[ Z_{N}^{B,F} = (\pm)^{N} \sum_{n_{1},n_{2},\ldots,n_{N}}^{N} \prod_{j=1}^{N} \frac{[\pm Z_{1}(j\beta)/j]^{n_{j}}}{n_{j}!} , \] (1)
where \( Z_{1}(\beta) \) is the single particle partition function, \( \beta \) is the inverse temperature and the upper and lower signs refer to bosons and fermions respectively. The sum over the set of integers \( n_{i} \) is constrained by the relation
\[ \sum_{j=1}^{N} jn_{j} = N . \] (2)
The above formula allows us to write a general recursion relationship for the canonical partition function
\[ Z_{N}^{B,F} = \frac{1}{N} \sum_{n=1}^{N} (\pm)^{n+1} Z_{1}(n\beta)Z_{N-n}^{B,F}(\beta) \] (3)
for bosons (+) and fermions (−). We note that in the above recursion relation \( Z_{0} \) is formally taken to be unity for consistency.

In order to perform explicit calculations, we specialise to the case of a harmonic oscillator in d-dimensions. The single particle partition function is given by,
\[ Z_{1}(\beta) = \left[ \frac{x^{1/2}}{(1-x)} \right]^{d} \] (4)
where
\[ x = e^{x(-\beta\hbar\omega)} . \] (5)
The canonical partition function for a system with \( N \) particles is then computed using Eq.(1) and is given by
\[ Z_{N} = x^{Nd/2} P_{N}(x) \prod_{j=1}^{N} \frac{1}{(1-x^{j})^{d}} , \] (6)
where \( P_{N}(x) \) is a polynomial in \( x \) which depends on the dimension and the statistics of the system. We shall use the notation \( P_{N}(x) = B_{N}(x) \) and \( P_{N}(x) = F_{N}(x) \) for bosons and Fermions where necessary. The polynomial may be calculated using the recursion relation in Eq.(4)
\[ P_{N}(x) = \frac{1}{N} \sum_{n=1}^{N} (\pm)^{n+1} \prod_{j=N-n+1}^{N} \frac{(1-x^{j})^{d}}{(1-x^{n})^{d}} P_{N-n}(x) . \] (7)
The recursion relation above should be used with the condition \( P_{0}(x) = 1 \) for both bosons and fermions. We further note that in one-dimension \( B_{N}(x) = 1 \) for bosons and \( F_{N}(x) = x^{N(N-1)/2} \) for fermions. They are however more complicated in higher dimensions [13].
A. Fluctuations from Microcanonical Counting

We first define the fluctuation in particle number from the ground state at a given excitation energy through a set of counting rules. Again we first write down the general formulae for a given set of discrete energy levels, and then specialize to the harmonic trap. The single particle partition function may be written as

\[ Z_1(\beta) = x^{\epsilon} \sum_{j=1}^{\infty} x^{\epsilon j}, \]

where \( x = e^{-\beta} \) and \( \epsilon_j, j = 0, \ldots, \infty \) are the single particle energies. It is understood that \( \beta \) in the exponent defining \( x \) has been multiplied by a characteristic energy scale of the system, and similarly \( \epsilon_j \) has been divided by the same, which we put to unity for convenience. For the harmonic oscillator, this energy scale is \( \hbar \omega \), and \( x \) is given by Eq.(5). Substituting this into Eq.(1), and expressing \( Z_N \) in a power series in \( x \), we obtain

\[ Z_N = x^{E_0} \sum_{k=1}^{\infty} \Omega(E_k^{(ex)}, N) x^{E_k^{(ex)}}, \]

where the \( N \)-particle eigen-energies \( E_k = E_0 + E_k^{(ex)} \) form an ordered set, with \( E_0 \) and \( E_k^{(ex)} \) denoting the ground state energy and the excitation energy with respect to the ground state respectively. The expansion coefficient \( \Omega(E_k^{(ex)}, N) \) denotes the number of possible ways of distributing the excitation energy \( E_k^{(ex)} \) in utmost \( N \) particles.

Furthermore we may write \( \Omega(E_k^{(ex)}, N) \) as

\[ \Omega(E_k^{(ex)}, N) = \sum_{N_{ex}=1}^{N} \omega(E_k^{(ex)}, N_{ex}, N) \]

where \( \omega(E_k^{(ex)}, N_{ex}, N) \) denotes the number of possible ways of distributing the excitation energy \( E_k^{(ex)} \) amongst exactly \( N_{ex} \) particles. Hence the probability of exciting exactly \( N_{ex} \) particles from an \( N \)-particle system at an excitation energy \( E_k^{(ex)} \) is given by

\[ p(E_k^{(ex)}, N_{ex}, N) = \frac{\omega(E_k^{(ex)}, N_{ex}, N)}{\Omega(E_k^{(ex)}, N)}, \quad N_{ex} = 0, \ldots, N. \]

By definition this probability is properly normalised. Further the probability has the following properties:

\[ p(0, N_{ex}, N) = \delta_{0N_{ex}}, \]

\[ p(E_k^{(ex)}, N_{ex}, N) = 0 \quad N_{ex} > N. \]

The number fluctuation in the ground state of the system may now be defined in terms of the moments of the probability distribution given above. We first define the moments:

\[ < N_{ex} > = \sum_{N_{ex}=1}^{N} N_{ex} p(E_k^{(ex)}, N_{ex}, N), \]

\[ < N_{ex}^2 > = \sum_{N_{ex}=1}^{N} N_{ex}^2 p(E_k^{(ex)}, N_{ex}, N), \]
and the number fluctuation from the ground state is given by,

$$
\delta N_0^2 = <N_{\text{ex}}^2> - <N_{\text{ex}}>^2 ,
\quad = <N_0^2> - <N_0>^2 ,
$$

(16)
since $<N_0> + <N_{\text{ex}}> = N$.

Few remarks are in order here: The above definitions apply equally well to bosonic and fermionic systems. The fluctuation in the number of particles from the ground state is expressed here as a function of the excitation energy with respect to the ground state. In the case of bosons this is just the fluctuation from the lowest energy single-particle state, where as for fermions it is the number fluctuation across the (zero temperature) Fermi energy. Formally the above expressions complete the necessary basic definitions for further analysis. In actual practice the counting of the number of possibilities to which a system may be excited is non-trivial. In the following, we give an example of bosons and fermions in a harmonic oscillator potential for the explicit calculation of $\omega(E_{k_{\text{ex}}^{(ex)}}, N_{\text{ex}}, N)$. Henceforth, we consider the excitation energy from the ground state to be $\hbar \omega$, and denote the corresponding microcanonical multiplicity to be $\omega(n, N_{\text{ex}}, N)$.

(a) Bosons in a $d$-dimensional harmonic oscillator.

In the case of a harmonic oscillator trap, all the single particle energy levels in a given shell have the same energy. The shell may be characterised by the index $k$ with energy $(k - 1 + d/2)\hbar \omega$, $k = 1, 2, \ldots \infty$, and degeneracy $g_k$. When the excitation energy is zero (equivalently at zero temperature) all the $N$ particles are in the ground state. Now consider exciting $N_{\text{ex}}$ particles from this ground state that share $n$ quanta of energy. Let there be $m_1$ bosons with 1 quantum of excitation energy, $m_2$ bosons with 2 quanta of excitation, and so on. We then have

$$
n = m_1 + 2m_2 + \ldots + (n + 1 - N_{\text{ex}})m_{N_{\text{ex}}}
$$

and

$$
N_{\text{ex}} = m_1 + m_2 + \ldots + m_{N_{\text{ex}}}.
$$

This is just a way of partitioning an integer $n$ into exactly $N_{\text{ex}}$ partitions with $m_i$ denoting the number of times an integer $i$ appears in a partition (it is taken to be zero if some integer between 1 and $n + 1 - N_{\text{ex}}$ does not appear in the partition). All the $m_i$ bosons occupy the state $i + 1$, since $i = 1$ is the ground state. The number of ways these $m_i$ bosons are distributed in the state $i + 1$ is given by the counting rule

$$
(g_i + m_i - 1)C_{m_i}.
$$

(17)
The set $\{m_i\}$ denotes the set of all partitions of $n$ for a given $N_{\text{ex}}$. The microcanonical distribution $\omega$ is then given by

$$
\omega(n, N_{\text{ex}}, N) = \sum_{\{m_k\}} \prod_{k=1}^{N_{\text{ex}}} (g_k + m_k - 1)C_{m_k}.
$$

(18)
The formula for $\omega$ is especially simple in one dimension since there is no degeneracy, $g_k = 1$ for all $k$. We have,
\[ \omega(n, N_{\text{ex}}, N) = \sum_{\{m_k\}} 1, \]  

and the number of possibilities are determined by the number of ways an integer \( n \) can be partitioned into \( N_{\text{ex}} \) integers, that is the number of ways we can write,

\[ n = n_1 + n_2 + n_3 + \ldots + n_{N_{\text{ex}}}, \quad n_1 \geq n_2 \geq \ldots \geq n_{N_{\text{ex}}}. \]

Once the \( \omega \)'s are known the probability distribution may be calculated using the Eq. (11) and hence the fluctuations as a function of the excitation energy. In order to express this as a function of temperature, one may use the relation between excitation energy above the ground state and the temperature to be discussed presently (see Eq. (23)). We, however, prefer to present all results as a function of the excitation energy only. Since \( N_{\text{ex}} \leq N \) always, we can give an alternative expression for \( \omega \) as

\[ \omega(n, N_{\text{ex}}, N) = \Omega(n, N_{\text{ex}}) - \Omega(n, N_{\text{ex}} - 1). \]  

While this allows an alternative and probably a simpler way of calculating probability distribution, it is valid only for bosons (see the discussion following Eq. (24) given later).

(b) Fermions in a harmonic-oscillator (closed shell).

For simplicity, the fermions are taken to be spinless, and filling an integral number of shells in the ground state. The determination of microcanonical distribution \( \omega(n, N_{\text{ex}}, N) \) is more involved than in the case of bosons. The combinatoric rules depend on the space dimension. Using the same notation for the harmonic oscillator single particle energies in a given shell, we calculate the number of possibilities by which \( N_{\text{ex}} \) particles can be excited from the ground state. Note that removing \( N_{\text{ex}} \) fermions from the ground state leaves as many holes in ground state. As a result the \( \omega \) depends not only on the distribution of fermions in the excited states (as in the case of bosons), but also on how the holes are distributed in the ground state. For simplicity we choose a completely closed shell system, the rules may be appropriately modified for open shells. We assume that \( N \) fermions form a closed-shell system at \( T = 0 \) with shells up to \( k \) (corresponding to fermi energy \( E_F = (k-1 + d/2)\hbar \omega \)) filled. Thus \( N_{\text{ex}} \) holes are distributed in states from \( i = 1 \) up to \( i = k \). Let \( h_i \) denote the number of holes in the state \( i \) such that

\[ N_{\text{ex}} = h_1 + h_2 + \ldots + h_k. \]

The number of ways \( h_i \) holes may be created in the \( i \)th state is given by \( g_i C_{h_i} \). Hence the number of ways in which \( N_{\text{ex}} \) holes may be created in the ground state is given by the product over the number of ways in which the holes may be distributed in the \( k \) orbitals, i.e.,

\[ \prod_{j=1}^{k} (g_j C_{h_j}). \]

Now consider exciting \( N_{\text{ex}} \) particles from this ground state sharing \( n \) quanta of energy. An allowed configuration is one in which each and every one of these \( N_{\text{ex}} \) particles is found in states above the fermi energy, with the shell indices ranging from \( (k + 1) \) up to \( (k + n) \), such that their excitation energies add up to yield the total \( E_{\text{ex}} \). This complicates the counting.
rules for fermions as compared to bosons. We shall denote the occupancy of orbitals for the excited particles by $m_i$, where $i = k + 1, ..., k + n$. The number of ways the $m_i$ fermions are distributed in the state $k + i$ is then given by the counting rule

$$(g_{k+i}) C_{m_i}.$$ 

The microcanonical distribution $\omega$ is then given by

$$\omega(n, N_{ex}, N) = \sum_{\{m_i\}} \sum_{\{h_j\}} \prod_{j=1}^{k} (g_j) C_{h_j} \prod_{i=k+1}^{k+n} (g_{k+i}) C_{m_i}, \quad (21)$$

where $N_{ex} = \sum_i m_i$, and the microcanonical multiplicity $\omega$ is obtained by summing over all the allowed possibilities such that the sum total of the excited quanta is exactly $n$. Once the $\omega$’s are known the probability distribution may be calculated using the Eq. (11) and hence the fluctuation as a function of the excitation energy.

We compare these results with the fluctuations obtained by the canonical ensemble averaging method of Parvan et al. \[12\] as detailed below. It is our objective to see how close are the results for the ground state fluctuations calculated by the two methods.

**B. Fluctuations from canonical ensemble averaging**

In statistical thermodynamics, a macro-state at a given energy may be built up by many combinatorial ways from the micro-states, and this is denoted by the term multiplicity of the macro-state. As we saw in the preceding sect. (II A), the multiplicity $\Omega(E_{ex}^k, N)$ was defined by Eq. (10) through this counting method. In the canonical ensemble, we may alternately define

$$\Omega(T, N) = \exp[S(T, N)] = \exp[(U - F)/T] = x^{-U Z_N(x)} . \quad (22)$$

In the above, the internal energy $U(T)$ is determined as usual from the canonical partition function, and excitation energy at any temperature is given by

$$E^{(ex)} = U(T) - U(0) . \quad (23)$$

We may therefore compare the calculated quantities from the canonical and the microcanonical ensembles as a function of the excitation energy.

Comparing $\Omega(T, N)$ given by Eq. (22) from the canonical ensemble with the series (9), we see that it is as if only one term from this series is picked in the ensemble averaging. This is realized for a large number of particles, since the multiplicity $\Omega(E_{ex}^k, N)$ increases rapidly with the excitation energy, where as the factor $x^{E_k}$ decreases exponentially. In this paper, we focus on systems where $N$ is not large, specially for fermions. It is therefore interesting to examine the differences in the results of the calculation made by the two methods.

Once the multiplicity $\Omega$ is obtained, the fluctuations may be defined through a temperature dependent probability distribution \[5, 6\],

$$p(T, N_{ex}, N) = \frac{\Omega(T, N_{ex}) - \Omega(T, N_{ex} - 1)}{\Omega(T, N)}, \quad N_x = 0, ..., N. \quad (24)$$
Note that $\Omega(T, N_{\text{ex}})$ is determined by the canonical partition function of $N_{\text{ex}}$ particles by replacing $N$ by $N_{\text{ex}}$ in Eq. (22). For bosons, the ground state of every such system consists of a single level, and the definition given by Eq. (24) is correct. For fermions, however, the Fermi energy of a system defined by $N_{\text{ex}}$ particles is less than the Fermi energy of the full system with $N$ particles. The fluctuations are defined with respect to the ground state with the Fermi energy corresponding to the full system. Therefore Eq. (24) cannot be applied to fermions. A consistent definition of ground state fluctuations applicable to both fermions and bosons, and which coincides for the bosonic calculation with the probability definition (24), may however be given by the ensemble averaging method [11,12]. We summarise the method below.

The canonical partition function in Eq. (9) may be written in the occupation number representation as [12]

$$Z_N = \sum_{\{n_k\}} \prod_k x^{\epsilon_k n_k}, \tag{25}$$

where we have used the fact that the energy of the $N$-particle system for a given set of occupancies $\{n_k\}$ is given by $E = \sum_k \epsilon_k n_k$. The occupancy $n_k = 0, 1$ for fermions and may take any value up to $N$ for bosons. At finite temperatures, using the recursion relation in Eq. (3), and some nontrivial algebra, the ensemble-averaged moments of the occupancy $n_k$ may be written as [12]

$$< n_k > = \frac{1}{Z_N} \sum_{j=1}^N (\pm)^{j+1} x^{j \epsilon_k} Z_{N-j}, \tag{26}$$

$$< n_k^2 > = \frac{1}{Z_N} \sum_{j=1}^N (\pm)^{j+1} j x^{j \epsilon_k} Z_{N-j} + \frac{1}{Z_N} \sum_{j=1}^N \sum_{i=1}^{N-j} (\pm)^{i+j} x^{(i+j) \epsilon_k} Z_{N-i-j}, \tag{27}$$

where the upper and lower signs refer to bosons and fermions respectively.

The ground state fluctuation is now given by,

$$\delta N_0^2 = \sum_k (< n_k^2 > - < n_k >^2). \tag{28}$$

The sum runs through all the allowed $k$ values in the ground state defined at zero temperature. Note that the moments of occupancy are defined without any reference to the ground state. The fluctuation is then obtained by summing over the single particle states occupied at zero temperature. In the counting method as outlined earlier, the fluctuations necessarily refer to the ground state.

Applying the above equations to a system of bosons in a harmonic trap, we get

$$< n_0 > = \frac{1}{Z_N} \sum_{j=1}^N x^{jd/2} Z_{N-j}, \tag{29}$$

$$< n_0^2 > = \frac{1}{Z_N} \sum_{j=1}^N (2j - 1) x^{jd/2} Z_{N-j}. \tag{30}$$
The ground state fluctuation is given by Eq.\:(28),
\[
\delta N_0^2 = (\langle n_0^2 \rangle - \langle n_0 \rangle^2).
\]

Similarly, the thermodynamic expression for the ground state fluctuations for the fermionic system in a harmonic oscillator is obtained from Eq.\:(26) and Eq.\:(27):
\[
\langle n_s \rangle = \frac{1}{Z_N} \sum_{j=1}^{N} (-1)^{j+1} g_s x^{j(s-1+d/2)} Z_{N-j}, \quad (32)
\]
\[
\langle n_s^2 \rangle = \frac{1}{Z_N} \sum_{j=1}^{N} (-1)^{j+1} (jg_s - (j-1)g_s^2)x^{j(s-1+d/2)} Z_{N-j}, \quad (33)
\]
where \(g_s\) refers to the degeneracy factor of the state \(s\). For the \(N\)-fermion system that forms a closed shell system at \(T = 0\) with filled shells up to \(k\), with Fermi energy \(E_F = (k - 1 + d/2)\hbar \omega\), the ground state fluctuation is given by Eq.\:(28):
\[
\delta N_0^2 = \sum_{s=1}^{k} (\langle n_s^2 \rangle - \langle n_s \rangle^2). \quad (34)
\]

Before using these formulae for the calculation of ground state occupancy and fluctuations, we discuss below the specially interesting case of the one-dimensional harmonic confinement where the canonical and the microcanonical ensembles yield vastly different results.

**III. FLUCTUATIONS IN A ONE-DIMENSIONAL HARMONIC TRAP**

The one-dimensional Harmonic trap is specially interesting because even though the canonical entropies for bosons and fermions are identical, the number fluctuations from the ground state are very different. This may be seen by writing the canonical \(N\)-particle partition function as
\[
Z_N = x^{gN(N-1)/2 + N/2} \prod_{j=1}^{N} \frac{1}{1-x^j}, \quad (35)
\]
with \(g = 0\) for bosons, and \(g = 1\) for fermions. Actually, for other positive values of \(g\), the above form is the exact partition function for the so-called Calogero-Sutherland model [10], where the \(N\) particles interact pair-wise by a potential \(\frac{\hbar^2}{m} \sum_{i<j}^N (x_i - x_j)^{-2}\). For bosons, the dimensionless parameter \(g\) is in the range \(0 \leq g \leq 1/2\), while for fermions \(g > 1/2\). The special values \(g = 1(0)\) give noninteracting fermions (bosons). The effect of interaction has only been to shift the energy of every state by the same amount, which is absorbed in the prefactor. It follows from Eqs.\:(3,35) that we may write
\[
Z_N = x^{gN(N-1)/2 + N/2} \sum_{n=0}^{\infty} \Omega(n, N)x^n, \quad (36)
\]
and that \(\Omega(n, N)\) is independent of the parameter \(g\), and is the same for bosons and fermions. Since it is the logarithm of \(\Omega(n, N)\) that determines the canonical entropy of the system at
an excitation energy of \( n \) quanta, it follows that the entropy is independent of \( g \). The same result is true if one calculates the ensemble averaged entropy at a given temperature. This may be easily verified by using the relation \( F = -\ln Z_N / \beta \) for the free energy, and then calculating the entropy \( S = -\frac{\partial F}{\partial T} \).

For the microcanonical calculation of the fluctuation, we need to calculate the microcanonical multiplicity \( \omega(n, N_{ex}, N) \), which is the number of ways of distributing the \( n \) excitation quanta amongst exactly \( N_{ex} \) particles. Although the relation

\[
\Omega(n, N) = \sum_{N_{ex}=1}^{N} \omega(n, N_{ex}, N) \quad (37)
\]

is obeyed both by fermions and bosons, and the LHS of the above equation is the same for both, the microcanonical counting of \( \omega \)'s are very different for the two cases. In the appendix, this is illustrated explicitly for \( N = 3 \). Thus the fluctuations for the bosonic and fermionic cases differ substantially when the exact counting method is used. As is to be expected, the fermionic fluctuation is considerably suppressed compared to the bosonic system. The same qualitative conclusion may also be reached by using Eqs.(30, 33) based on canonical ensemble averaging rather than exact counting. In the next section, we display these results, as well as the results for the two-dimensional harmonic oscillator.

**IV. RESULTS AND DISCUSSION**

In Fig.(1), we display (a) the ground state occupancy \( <N_0> \) and (b) the relative fluctuation \( <\delta N_0>/N \) for \( N = 15 \) noninteracting particles in a one-dimensional harmonic oscillator potential. The canonical and the exact microcanonical results are compared as a function of the excitation energy. The canonical method gives results in close agreement with counting for the ground state occupancy \( <N_0> \), but overestimates the relative fluctuation substantially. In one dimension, the number of microcanonical possibilities \( \omega(n, N_{ex}, N) \) is very restricted at low excitations due to the non-degeneracy in the single-particle energy levels and the Pauli exclusion principle. This results in (i) \( <N_0> \) for fermions getting depleted more slowly than bosons, and (ii) reduced fluctuation. In Fig.(2), the same quantities are displayed for particles in a two-dimensional harmonic oscillator potential. It is well known from previous work \([5–7]\) that there is a peak in the relative fluctuation somewhat below the critical temperature for bosons. For fermions, such peaking is absent, specially in the exact calculation. We thus see that the presence or absence of a peak in the number fluctuation of the ground state may signal phase transition, or its absence.

The microcanonical method of exact counting for fermions is computationally very time-consuming because, unlike bosons, Eq.(24) cannot be used. We have therefore restricted the fermionic calculations to only up to \( N = 15 \) particles. As we see from Figs (1-2), there is considerable difference in the results for the relative fluctuations for small particle numbers. For fermions, we expect this difference to persist at low excitations even when \( N \) is large. This is because at low excitations, only a small fraction of the fermions near the Fermi sea can be excited, so the effective number of fermions contributing to the number fluctuation remains small even when the system is large. For bosons, there is no difficulty in performing the microcanonical calculation for a large number of particles. In Fig.(3),
we show the bosonic occupancy and the relative fluctuation as a function of the number of excitation quanta for $N = 100$. We note that the occupancy $< N_0 >$ from the canonical and exact microcanonical methods is practically identical, although the ground state fluctuation continue to differ.

We have made the comparison between the microcanonical and canonical results as functions of the excitation energy, rather than temperature. In the microcanonical method, the counting of the possibilities is done for a given excitation energy, the latter being the natural variable. In the canonical formalism, of course, a mapping from the excitation energy to temperature can be done using Eq.(23). We may also note that starting from the canonical Eq.(22) and using Eq.(24) for bosons, one can obtain the analytical expression for the low temperature dependence of the fluctuation, as, for example, given by Eq.(14) of [3]. It remains a challenging problem to obtain similar microcanonical relations for fermions.

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FIGURES

FIG. 1. (a) Plots of the ground state occupancy $< N_0 >$ versus the excitation energy $E_{ex}$ for $N = 15$ bosons (fermions) in a one-dimensional harmonic oscillator. $E_{ex}$ is given in units of the oscillator spacing. The microcanonical results are displayed according to the legends in the inset box. (b) Plots of the relative ground state fluctuation $< \delta N_0 > / N$ as a function of $E_{ex}$ for the same systems as in (a).

FIG. 2. (a) Plots of the ground state occupancy $< N_0 >$ versus the excitation energy $E_{ex}$ for $N = 10$ bosons (fermions) in a two-dimensional harmonic oscillator, according to the legends in the inset box. (b) Plots of the relative ground state fluctuation $< \delta N_0 > / N$ as a function of $E_{ex}$ for the same systems as in (a).

FIG. 3. (a) Plots of the ground state occupancy $< N_0 >$ versus the excitation energy $E_{ex}$ for $N = 100$ bosons in a one-dimensional harmonic oscillator. (b) Plots of the relative ground state fluctuation $< \delta N_0 > / N$ as a function of $E_{ex}$ for the same system as in (a).
V. APPENDIX

Calculation of \( \omega(n, N_{ex}, N) \) in one-dimensional harmonic oscillator.

(a) **Bosons**

For illustration, in Table 1, we display the simple case of \( N = 3 \) bosons, with the number of excitation quanta \( n \leq 7 \). Since there is no degeneracy, the combinatorial factor given by \( (17) \) is unity. Therefore \( \omega(n, N_{ex}, N) \) in this case is just the number of distinct ways in which the integer \( n \) may be partitioned amongst exactly \( N_{ex} \) identical bosons (\( N_{ex} \leq 3 \)). In Table 1, \( n \) increases from left to right, and increasing values of \( N_{ex} \) are tabulated in a vertical column. The integer in each box is the corresponding \( \omega(n, N_{ex}, N) \), with the distinct partitions of \( n \) listed in brackets below it. For example, in the box under \( (n = 4, N_{ex} = 2) \), we see that \( \omega(4, 2, 3) = 2 \), and the two distinct partitions of 4 are \((3 + 1)\) and \((2 + 2)\). In the last row is listed \( \Omega(n, N) \), that is obtained by adding the \( \omega(n, N_{ex}, N) \)'s in each vertical column. Note that these check with the coefficients in the expansion of the 3-boson canonical partition function:

\[
Z_3 = 1 + x + 2x^2 + 3x^3 + 4x^4 + 5x^5 + 7x^6 + 8x^7 + \ldots
\]

(b) **Fermions**

Same as for bosons, except that two more vertical columns have been added under the headings \( L_1 \) and \( n_{min} \). For three spinless fermions, the lowest three energy levels \((1, 2, 3)\) (in increasing order of energy) are occupied at \( T = 0 \). The column under \( L_1 \) lists the possible configuration of holes in these levels for an excitation energy of \( n \geq n_{min} \) quanta, the latter being listed in the adjacent column. For example, for \( N_{ex} = 2 \), \((312_1)\) under the column \( L_1 \) denotes a two-hole configuration, with one hole in level 3, and another in level 2. The minimum energy required for this is \( n_{min} = 4 \) in units of \( \hbar \omega \).
TABLES

**TABLE I. Tabulation of bosonic $\omega(n, N_{ex}, N)$ for $N=3$**

| $n$ | $N_{ex} = 1$ | $N_{ex} = 2$ | $N_{ex} = 3$ |
|-----|--------------|--------------|--------------|
|     | 1            | 2            | 3            |
| $N_{ex} = 1$ | 1            | 1            | 1            |
| $N_{ex} = 2$ | 0            | 0            | 0            |
| $N_{ex} = 3$ | 0            | 0            | 0            |
| $\omega(n, N_{ex}, N)$ | 1 (1+1) | 1 (2+1) | 1 (1+1+1) |
|     | 1 (3+1) | 1 (2+1+1) | 2 (3+1+1) |
|     | 2 (4+1) | 2 (2+2+1) | 3 (2+2+1) |
|     | 3 (5+1) | 3 (3+2+1) | 4 (3+3+1) |
|     | 3 (6+1) | 3 (4+2+1) | (3+2+2) |
| $\Omega(n, N) =$ | 1 | 2 | 3 |

**TABLE II. Tabulation of fermionic $\omega(n, N_{ex}, N)$ for $N=3$**

| $n$ | $n_{min}$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|-----|-----------|---|---|---|---|---|---|---|
| $N_{ex} = 1$ : | 3_1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
|     | 2_1 | 2 | 0 | 1 | 1 | 1 | 1 | 1 |
|     | 1_1 | 3 | 0 | 0 | 1 | 1 | 1 | 1 |
| $\omega(n, 1, N) =$ | 1 | 2 | 3 | 3 | 3 | 3 | 3 |
| $N_{ex} = 2$ : | 3_1 2_1 | 4 | 0 | 0 | 0 | 1 (1+3) | 1 (1+4) | 2 (1+5) | 2 (1+6) |
|     | 3_1 1_1 | 5 | 0 | 0 | 0 | 0 | 1 (1+4) | 1 (1+5) | 2 (1+6) |
|     | 2_1 1_1 | 6 | 0 | 0 | 0 | 0 | 0 | 1 (2+4) | 1 (2+5) |
| $\omega(n, 2, N) =$ | 0 | 0 | 0 | 1 | 2 | 4 | 5 |
| $N_{ex} = 3$ : | 3_1 2_1 1_1 | 9 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\omega(n, 3, N) =$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\Omega(n, N) =$ | 1 | 2 | 3 | 4 | 5 | 7 | 8 |
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fig1a: 1DHO, N=15
fig1b: 1DHO, N=15

- B–Canonical Ensemble
- F–Canonical Ensemble
- B–Counting Rule
- F–Counting Rule
fig2a: 2DHO, N=10

The figure shows the relationship between $E_{ex}$ and $\hat{N}$/\sqrt{\nu}$ for a 2D Harmonic Oscillator with $N=10$. The graph includes data points and lines for different ensemble types:

- **B-Canonical Ensemble**
- **F-Canonical Ensemble**
- **B-Counting Rule**
- **F-Counting Rule**
fig2b: 2DHO, N=10

- B—Canonical Ensemble
- F—Canonical Ensemble
- B—Counting Rule
- F—Counting Rule
fig3a: 1DHO, N=100

B–Canonical Ensemble
B–Counting Rule
fig3b: 1DHO, N=100

$\langle \delta \frac{N_0}{N} \rangle$ vs $E_{ex}$

- B-Canonical Ensemble
- B-Counting Rule