Ground State Number Fluctuations of Trapped Particles

by

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Abstract

This thesis encompasses a number of problems related to the number fluctuations from the ground state of ideal particles in different statistical ensembles. In the microcanonical ensemble most of these problems may be solved using number theory. Given an energy E, the well-known problem of finding the number of ways of distributing N bosons over the excited levels of a one-dimensional harmonic spectrum, for instance, is equivalent to the number of restricted partitions of E. As a result, the number fluctuation from the ground state in the microcanonical ensemble for this system may be found analytically. When the particles are fermions instead of bosons, however, it is difficult to calculate the exact ground state number fluctuation because the fermionic ground state consists of many levels. By breaking up the energy spectrum into particle and hole sectors, and mapping the problem onto the classic number partitioning theory, we formulate a method of calculating the particle number fluctuation from the ground state in the microcanonical ensemble for fermions. The same quantity is calculated for particles interacting via an inverse-square pairwise interaction in one dimension. In the canonical ensemble, an analytical formula for the ground state number fluctuation is obtained by using the mapping of this system onto a system of noninteracting particles obeying the Haldane-Wu exclusion statistics. In the microcanonical ensemble, however, the result can be obtained only for a limited set of values of the interacting strength parameter.

Usually, for a discrete set of a mean-field single-particle quantum spectrum and in the microcanonical ensemble, there are many combinations of exciting particles from the ground state. The spectrum given by the logarithms of the prime number sequence, however, is a counterexample to this rule. Here, as a consequence of the fundamental theorem of arithmetic, there is a one-to-one correspondence between the microstate and the macrostate, resulting in the vanishing of number fluctuation for all excitations. The use of the canonical or grand canonical ensembles, on the other hand, gives a substantial number fluctuation from the ground state. For a related spectrum, that given by the logarithms of

an integer n, the microcanonical number fluctuation is non-zero but the application of the other ensembles is still not valid. These two spectra are examples of systems where canonical and grand canonical ensembles averagings yield answers different from the microcanonical result.

Some models in physics may be used to obtain formulae known in the theory of number partition. For the same problem of N ideal bosons in a one-dimensional harmonic oscillator potential mentioned earlier, it is well known that the asymptotic ($\mathrm{N} \to \infty$) density of states is identical to the Hardy-Ramanujan formula for the number of partitions of an integer n. The same statistical mechanics technique for the density of states of bosons in a power-law spectrum yields the partitioning formula for the number of partitions of n into a sum of sth powers of a set of integers. By considering only the particle sector of the fermionic spectrum, a formula for the number of distinct partitions of n is obtained. For the $s = 1$ case and for finite N, the Erdos-Lehner formula for the restricted partitions, and a new formula for the distinct and restricted partitions are derived.

As a diversion, we discuss the microcanonical entropy which may be uniquely defined in terms of the macrostate, or equivalently the many-body degeneracy of the state, at a given energy. The many-body degeneracy factor, however, is exceedingly difficult to calculate in general. It is thus desirable to find a different way to calculate the microcanonical entropy. It has been recently suggested that the microcanonical entropy may be accurately reproduced by including a logarithmic correction to the canonical entropy. This claim is readily tested using some of the models mentioned above, where the many-body degeneracy may be determined exactly. In addition, we also consider a system of N distinguishable particles in a d-dimensional harmonic energy spectrum. In this case the many-body degeneracy factor can be obtained analytically in a closed form.

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Contents

Chapter 1

Introduction

"The beginning is the most important part of the work."
Plato (427-347 BC), The Republic

In the last two decades there have been tremendous advances in the experiments of trapping atoms. Following the experimental discovery of Bose-Einstein condensation (BEC) of trapped atoms in 1995, the ideal Bose gas has been attracting considerable theoretical interest with a wide range of topics. One such topic is the number fluctuation from the ground state, discussed in this thesis. Here, we focus on systems of particles which are essentially noninteracting in different traps. For the most part, these systems have an interesting link to number theory.

1.1 Review of Previous Work

Some aspects of the work in this thesis are a continuation of previous work, which in turn was motivated by the problem of number fluctuation of a system of Bose gas. In standard statistical mechanics, the usual textbook approach is based on the grand canonical ensemble (GCE). The number fluctuation is found to be related to density-density correlation, and to the thermal compressibility of the system [1]. A connection between the ground state number fluctuation and the cross section for light scattering off a BEC has been proposed [2]. It is well known that the standard expression for the number fluctuation of Bose gas in the GCE is divergent at low temperatures [1, 3, 4, 5]. This expression is given by

$$\langle \triangle n_i^2 \rangle = \langle n_i \rangle \left(1 + \langle n_i \rangle\right), \tag{1.1}$$

where $\langle n_i \rangle = (e^{(\epsilon_i - \mu)\beta} - 1)^{-1}$ is the average occupation with energy ϵ_i at temperature $k_B T = 1/\beta$, and μ is the chemical potential. As the temperature of the system approaches zero, the average occupancy of the excited states becomes small while that of the ground state becomes macroscopic, and approaches N, the total number of particles. Using the above formula, the *ground state number fluctuation* is thus $\langle \triangle N_0 \rangle \approx \langle N \rangle$ which is clearly nonphysical since the number fluctuation should vanish at zero temperature. In an attempt to overcome this problem, the authors in Ref. [4] proposed instead $\langle \triangle {N_0}^2 \rangle / N^2 \rightarrow (N/\langle N_0 \rangle - 1)^2$ which goes to zero with temperature. Recall that the GCE allows particle exchange between the system and its surrounding. However, in the experimental setting of BEC in a trapped dilute gas at ultra-low temperatures [6, 7, 8], the number of particles does not fluctuate when the cooling process is over. It is therefore more appropriate to calculate the ground state number fluctuation within the canonical ensemble (CE), or the microcanonical ensemble (MCE) formalism (a detailed discussion of the different ensembles is given in section 2.1).

To have an understanding of what the fluctuation of the ground state occupancy number means, consider a simple example given in the figure below. We assume the particles are noninteracting bosons. The single-particle energy spectrum is taken to be harmonic, $\epsilon_n = n$, and the total number of particles $N = 3$. At $T = 0$, all the particles reside in the lowest state. For a given fixed excitation energy E_{ex}, in this case $E_{ex} = 5$, there are many ways the particles can share this energy and be excited to the higher levels. The number of ground state particles does not remain constant and thus fluctuates as a function of excitation energy.

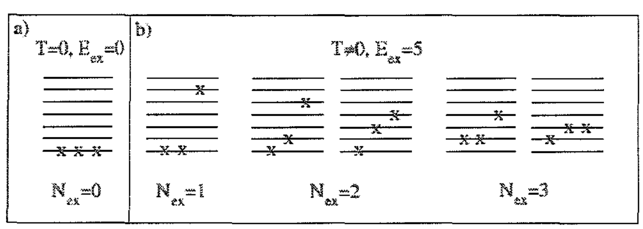


Figure 1.1: Illustration of the ground state number fluctuation for a one-dimensional harmonic trap. a) The system is at zero temperature, all the particles are in the ground state. b) Given an excitation energy $E_{ex} = 5$, there are many ways for the particles to share this energy. The number excited particles, N_{ex}, may vary from 1 to N. Note that the higher energy levels are not shown.

The calculation of the microcanonical ground state number fluctuation for ideal bose gas confined in a one-dimensional harmonic trap has been done analytically [9] in the limit of large N. For higher dimensions the results were obtained using approximate methods. In all cases the fluctuation of the ground state occupancy number were shown to vanish at zero temperature when either the CE or the MCE is used [9, 10, 11, 12, 13, 14, 15, 16, 17, 18]. Using different methods of approximation, the number fluctuation was also considered for weakly interacting bose gas [19, 20, 21, 22, 23, 24].

The microcanonical or canonical approach is in general very difficult. For ideal bosons in a one-dimensional harmonic trap, the problem is greatly simplified due to the connection to number partitioning theory [9]. A direct connection to number theory was not possible for ideal fermions, however, due to the fact that the fermionic ground state consists of many levels. In our previous work, we formulated a method for calculating the exact microcanonical fluctuation using combinatorics for ideal bosons and fermions as a function of excitation energy [25, 26]. Comparisons between the different ensembles were also made. The work on fermions was inspired by the experimental observation of quantum degeneracy in trapped fermionic gas at low temperatures by the authors in Ref. [27, 28]. The combinatorics method is, however, very time-consuming computationally. One of the objectives of the present work is to formulate an efficient method, using results from number theory similar to the bosonic case, to calculate the ground state number fluctuation for ideal spinless fermions. In the presence of interaction, the difficulty is greatly increased, even in the GCE. However, for certain kind of interaction, this can be done analytically [29]. One other objective of the present work is to calculate the number fluctuation of interacting particles in the CE and MCE.

1.2 Scope of the Present Work

The present work was in fact set out with the two main objectives mentioned earlier, namely, to effectively calculate the fermionic number fluctuation in the MCE and to find the fluctuation for interacting particles in the CE and MCE. During the research, the results of which were reported in Refs. [24, 30], some related questions were raised and induced more work. Therefore, this thesis may be thought of as a collection of results that are interconnected. For this reason, the next chapter is devoted to introducing some of the ideas in statistical physics and number theory necessary to the rest of the thesis. Chapter 2 thus serves to prepare the background for the subsequent chapters, and presents an overview of the ground state number fluctuation in different ensembles. Certain quantities in a many-body quantum system and their connection to the generating functions, found in the theory of number partitioning, are also discussed.

In Ref. [24] we calculated the number fluctuations for particles interacting via a two-body inverse square potential in one dimension, and a contact delta potential in two dimensions. At this point the calculations were only done in the GCE and CE. In the second part of Ref. [30], we carried on the work on interacting particles in one dimension and in the MCE. This was however possible only for a few values of the interaction strength parameter. We present these results on interacting particles in chapter 5. In the first part of Ref. [30], we reported a method for calculating the exact ground state number fluctuation for ideal fermions. By dividing the fermionic energy spectrum into hole and particle sectors, we were able to use results from the theory of number partition to greatly simplify the fermionic problem.

The one-dimensional harmonic trap is one of the many examples that illustrates an interesting link between physics and additive number theory. In fact, connections between statistical mechanics and additive number theory have been recognized for a long time (see *e.g.*, [31, 32]). Over the past decade, however, there have been theoretical works on newly connecting physical systems to *multiplicative* number theory. Julia [33, 34], for example, defined the so-called Riemann gas with the Riemann zeta function as its partition function. The zeta function was also used as partition function by Knauf [35] in his work on one-dimensional spin chains, and by Fivel [36] in connection to quantum entanglement. Recently, Boos *et al.* [37] showed that the correlations function in spin-1/2 Heisenberg XXX antiferromagnet can be expressed in terms of the values of Riemann zeta function at odd arguments. These are only a small number of examples, a more complete listing with the relevant publications may be found on line at www.maths.ex.ac.uk/∼mwatkins/zeta/surprising.htm.

After the successful application of additive number theory to calculate the exact ground state number fluctuation for fermions, we examine different systems that have links to multiplicative number theory. Noninteracting particles in traps with energy spectra given by $\ln p$ where p is prime, and $\ln n$ where n is integer, belong to this category. Using the fundamental theorem of arithmetic, the number fluctuation and the entropy in the first model is found to vanish *for all excitation energy* in the MCE [38]. Though the same remarkable outcome does hold for the $\ln n$ model, it nevertheless exhibits some other interesting characteristics. Both of these models are counterexamples to the principle of thermodynamic equivalence. This and the work on ideal fermions in the one-dimensional harmonic spectrum are presented in chapter 4, where we discuss number fluctuation of non-interacting particles. Also discussed in chapter 4 is the correction to the canonical entropy to obtain a formula that approximates the microcanonical entropy. Given N particles in a mean-field single-particle energy spectrum, the microcanonical entropy is given by the logarithm of the multiplicity of states. This quantity is in general difficult to find. On the other hand, the canonical entropy is relatively easier to determine once the partition function is known. If the quantum fluctuations are neglected, the microcanonical entropy may be obtained by subtracting a term involving energy fluctuations from the canonical value [39, 40, 41]. Previous to our work in [41], a special case of this formula was applied to the Bekenstein-Hawking Area Law (BHAL). In the last part of chapter 4, we derive the formula more generally, and test it for three different models where the multiplicity of states may be exactly found.

Chapter 3 is devoted to finding asymptotic formulae for different types of number of partitions of an integer n using methods of statistical mechanics. It is already well known that the Hardy-Ramanujan formula [42], which pertains to the number of partitions of n, is identical to the density of states of a system of bosons in a one-dimensional harmonic oscillator potential. The fermionic problem mentioned earlier, with the hole sector removed, bears close resemblance to the unrestricted but *distinct* number partition due to the Pauli principle. Some results and ideas from this work are used to derive an asymptotic formula for the number of partitions of n into a sum of s^{th} powers of a set of distinct integers $\leq n$. In addition, we also derive asymptotic formulae for partitioning an integer n into a sum of s^{th} powers of other integers, where the integers need not be distinct. In both cases the size of the set of integers may be unrestricted or restricted. The formula for the unrestricted partitions with $s = 1$ reduces to Hardy-Ramanujan formula [42], and that for the restricted partitions to the Erdos-Lehner formula [43].

Finally, in chapter 6 we summarize the main results presented in this thesis. In addition, we also discuss some questions yet to be addressed. As is the story of this thesis, the quest for the answers to these questions might induce more future research.

Chapter 2

Preliminaries

*" All intelligent thoughts have already been thought;
what is necessary is only to try to think them again."*
Johann Wolfgang von Goethe (1749-1832)

Most of the concepts and techniques used in this work are quite basic and require no more than fundamental knowledge in quantum statistical mechanics. They are, however, essential tools for uncovering many results reported in this thesis. We review and summarize some of the methodologies which shall be constantly used in this thesis. It must be noted that these theories are by no means complete, but are presented in such a way that enables one to apply them directly in this work. Section 2.1 discusses the ground state number fluctuation in different ensembles in statistical mechanics. Section 2.2 discusses the quantum degeneracy and the quantum density of states. Finally, section 2.3 introduces the so-called generating functions, which are found in additive number theory, and which are largely accountable for the work in chapter 3. Note that in all the treatments here the particles are assumed to be noninteracting. This might be regarded as an independent-particle picture, or a mean field picture in which the quasiparticles are noninteracting.

2.1 The Different Ensembles

2.1.1 The microcanonical ensemble

The concept of an ensemble is an important idea in statistical mechanics. The first ensemble considered is called the *microcanonical ensemble* (MCE) following the nomenclature introduced by Williard Gibbs. It is a collection of similar systems all prepared identically with the same number of particles, energy, volume, shape, magnetic field, etc. All the systems are isolated from one another, such that the energy and the number of particles of each system are fixed. To be concrete, consider the example in section 1.1, whose quantum spectrum is shown in Fig. 1.1. This system is completely isolated from the surrounding. Defining the microstate $\omega(E_{ex}, N_{ex}, N)$ to be the number of ways of exciting N_{ex} particles given an excitation energy E_{ex}, then the probability of doing this is

$$P(E_{ex}, N_{ex}, N) = C\ \omega(E_{ex}, N_{ex}, N), \tag{2.1}$$

where C is the normalization constant determined by

$$1 = \sum_{N_{ex}=1}^{N} P(E_{ex}, N_{ex}, N) = C \sum_{N_{ex}=1}^{N} \omega(E_{ex}, N_{ex}, N).$$

Therefore,

$$C = \frac{1}{\sum \omega(E_{ex}, N_{ex}, N)} = \frac{1}{\Omega(E_{ex}, N)},$$

where

$$\Omega(E_{ex}, N) \equiv \sum_{N_{ex}=1}^{N} \omega(E_{ex}, N_{ex}, N) \tag{2.2}$$

is the macrostate or equivalently, the multiplicity of the quantum states having the same energy. We shall see that this is identical to the degeneracy of the many-body energy level with eigenvalue E_n, where $\{E_n\}$ is the many-body quantum spectrum. The meaning of this quantity with respect to a many-body system shall be more clear as we discuss it in more detail in section 2.2.1. For now, it is sufficient to interpret it as a sum of the microstates as given by Eq. (2.2). From Fig. 1.1, $\Omega(E_{ex}, N) = \Omega(5,3) = 5$, and the corresponding probabilities are

$$P(5,1,3) = \frac{1}{5},$$

$$P(5,2,3) = \frac{2}{5},$$

and

$$P(5,3,3) = \frac{2}{5}.$$

The first and second moments of the excited particles may be determined using

$$\langle N_{ex} \rangle = \sum_{N_{ex}=1}^{N} N_{ex}\ P(E_{ex}, N_{ex}, N), \tag{2.3}$$

$$\langle {N_{ex}}^2 \rangle = \sum_{N_{ex}=1}^{N} {N_{ex}}^2\ P(E_{ex}, N_{ex}, N), \tag{2.4}$$

where $N = 3$ in the example. The ground state number fluctuation, by definition, reads

$$\left\langle \triangle N_0{}^2 \right\rangle = \left\langle N_0{}^2 \right\rangle - \left\langle N_0 \right\rangle^2 , \tag{2.5}$$

where N_0 is the number of particles in the ground state. We need, however, to express $\left\langle \triangle N_0{}^2 \right\rangle$ in terms of $\langle N_{ex} \rangle$ and $\left\langle N_{ex}{}^2 \right\rangle$. Note that since the system is completely isolated, the total number of particles N in the system is fixed, while N_0 and N_{ex} may vary such that

$$N = \langle N_0 \rangle + \langle N_{ex} \rangle . \tag{2.6}$$

Using Eq. (2.6), the ground state number fluctuation may be rewritten in terms of $\langle N_{ex} \rangle$ and $\left\langle N_{ex}{}^2 \right\rangle$ as

$$\begin{aligned} \left\langle \triangle N_0{}^2 \right\rangle &= \left\langle N_0{}^2 \right\rangle - \left\langle N_0 \right\rangle^2 , \\ &= \left\langle (N - N_{ex})^2 \right\rangle - (N - \langle N_{ex} \rangle)^2 , \\ &= \left(N^2 - 2N \langle N_{ex} \rangle + \left\langle N_{ex}{}^2 \right\rangle\right) - \left(N^2 - 2N \langle N_{ex} \rangle + \langle N_{ex} \rangle^2\right) , \\ &= \left\langle N_{ex}{}^2 \right\rangle - \langle N_{ex} \rangle^2 . \end{aligned} \tag{2.7}$$

It can clearly be seen that the whole problem of calculating the microcanonical ground state number fluctuation rests in finding the exact microstate $\omega(E, N_{ex}, N)$ and the macrostate $\Omega(E, N)$. In general, however, finding these two quantities is a difficult enterprise for large E and N. We shall see that depending on the symmetry of the problem, there are simpler means to obtain the macrostate $\Omega(E, N)$ from which the microstate $\omega(E, N_{ex}, N)$ and the ground state number fluctuation may be found.

2.1.2 The canonical ensemble

When the system considered in the previous section is put in a heat bath, the resulting ensemble is called the *canonical ensemble* (CE). The system and the heat bath are now in thermal contact such that heat is allowed to transfer from one to another. Therefore the energy of the system fluctuates. The system and the heat bath eventually reach thermal equilibrium at a temperature T. It is important to note that the only difference between the CE and the MCE is that heat transport is now allowed. The total number of particles of each system is fixed since particle transport is still prohibited in both ensembles.

The formulae given in section 2.1.1 no longer apply here since one of the constraints is now relaxed. The treatment in the CE, to be presented in this section, might seem more involved mathematically and less straightforward in appearance compared to the MCE. However, the determination of some thermodynamics quantities are computationally more feasible. In general the less number of constraints there is in a given system, the more feasible the calculations are.

We start with a many-body quantum mechanical system which is in contact with a heat reservoir and whose eigenenergy spectrum is described by a set of $\{E_n\}$. The probability for the system to be in the state with the energy eigenvalue E_n is

$$P_n = \frac{e^{-\beta E_n}}{Z_N}, \tag{2.8}$$

$\beta = 1/k_B T$ is the inverse temperature, k_B is the Boltzmann constant. For simplicity we shall put k_B to be unity. Eq. (2.8) is called the Boltzmann probability distribution. The quantity Z_N is determined from the normalization condition and is given by

$$Z_N = \sum_n e^{-\beta E_n}. \tag{2.9}$$

We have attached a subscript 'N' in Z_N to emphasize the many-body nature of the system considered. It must be stressed that the sum on the RHS of Eq. (2.9) is a sum *over states and not over energy eigenvalues* E_n. In general there may be more than one state for a given eigenenergy. The symbol Z is an abbreviation of the German word 'Zustandssumme', which means 'sum over states'. This quantity is called the *partition function* and is of utmost importance in statistical mechanics. Its importance arises because it enables one to make a connection between the quantum states of the system and its thermodynamic properties, such as the free energy, the entropy, etc. To see this, we start with the definition of the entropy [44]:

$$S_N = -\sum_n P_n \ \ln \ P_n. \tag{2.10}$$

Using Eq. (2.8),

$$\begin{aligned} S_N &= \sum_n P_n \ (\beta E_n + \ln Z_N), \\ &= \beta \sum_n P_n \ E_n + \ln Z_N, \\ &= \beta E + \ln Z_N, \end{aligned} \tag{2.11}$$

where E is the mean energy of the system, and we have used the fact that $\sum P_n = 1$ in the above. Eq. (2.11) can be rearranged to give

$$
\begin{aligned}
-\frac{1}{\beta}\ln Z_N &= E - \frac{1}{\beta}S_N, \\
&= F_N,
\end{aligned} \tag{2.12}
$$

which gives a relationship between the free energy F_N and the partition function $Z_N = e^{-\beta F_N}$.

The partition function Z_N may be alternatively expressed as a sum *over eigenenergy level* E_n instead of summing over states. If there are $\Omega(E_n, N)$ quantum states all with energy E_n, then Z_N may be written as

$$
Z_N = \sum_{E_n} \Omega(E_n, N) e^{-\beta E_n}, \tag{2.13}
$$

where the sum now is over the eigenenergy levels, and $\Omega(E_n, N)$ is the many-body quantum degeneracy of the level with energy eigenvalue E_n. This is the same quantity as given by Eq. (2.2) and which, as already mentioned, shall be discussed in more detail in section 2.2.1. It is difficult, or even impossible to find a closed form of Z_N. There are two cases where the many-body partition function is trivial. In the first case the particles are classical and distinguishable, the partition function reads

$$
Z_N = Z_1^N, \tag{2.14}
$$

where Z_1 is the partition function for a single particle:

$$
Z_1 = \sum_i e^{-\beta\epsilon_i}. \tag{2.15}
$$

In the above, $\{\epsilon_i\}$ is the single-particle eigenenergy spectrum, and the sum is again over states. Similar to Z_N, Z_1 may also be expressed as a sum over eigenenergy in which case the degeneracy factor of the level with eigenenergy value ϵ_i must be included. In the second case the particles are classical but indistinguishable (Boltzmann particles), and

$$
Z_N = \frac{Z_1^N}{N!}. \tag{2.16}
$$

In quantum statistics the particles are either bosons or fermions and are indistinguishable. A recipe for calculating the many-body partition function for these particles, assumed to be noninteracting, is given by [45]:

$$
Z_N(\beta) = \frac{1}{N}\sum_{j=1}^{N} \ (\pm)^{j+1} Z_1\,(j\beta)\, Z_{N-j}(\beta), \ \ Z_0(\beta) = 1, \tag{2.17}
$$

where (+) is for bosons and (-) for fermions.

One of the quantities that we are interested in is the ground state number fluctuation for both bosons and fermions. As will be clarified in section 2.2.1, for noninteracting particles the N-body problem pertains to filling up N particles in the single-particle energy levels ϵ_k. The first and second moments of the occupation number of the energy level k may be expressed in terms of the N-particle partition function as [46, 47]:

$$\begin{aligned} \langle n_k \rangle &= \frac{1}{Z_N} \sum_{j=1}^{N} (\pm)^{j+1} e^{-j\beta\epsilon_k} Z_{N-j}, && (2.18) \\ \langle n_k^2 \rangle &= \frac{1}{Z_N} \sum_{j=1}^{N} (\pm)^{j+1} [j \pm (j-1)] e^{-j\beta\epsilon_k} Z_{N-j}. && (2.19) \end{aligned}$$

Detailed derivations of Eqs. (2.18) and (2.19) are given in appendix A. The ground state number fluctuations for bosons, in terms of the occupation number, are simply

$$\langle \triangle N_0{}^2 \rangle = \langle n_0^2 \rangle - \langle n_0 \rangle^2, \tag{2.20}$$

and for fermions,

$$\begin{aligned} \langle \triangle N_0{}^2 \rangle &= \sum_k \left(\langle n_k^2 \rangle - \langle n_k \rangle^2 \right), \\ &= \sum_k \left(\langle n_k \rangle - \langle n_k \rangle^2 \right), \\ &= \sum_k \langle n_k \rangle \left((1 - \langle n_k \rangle \right). && (2.21) \end{aligned}$$

The sum k runs over all levels defining the fermionic ground state at zero temperature. In Eq. (2.21) we have used the identity $\langle n_k^2 \rangle = \langle n_k \rangle$ (see appendix A). The ground state number fluctuation for fermions may thus be determined solely from the knowledge of the first moment. It must be noted that Eqs. (2.20) and (2.21) are general and not restricted to the CE. The exact form of $\langle n_i \rangle$ and $\langle n_i^2 \rangle$ are, however, dependent on the ensembles used.

2.1.3 The grand canonical ensemble

In section 2.1.1 we considered the MCE where the system is completely isolated, while in section 2.1.2 it is allowed to be in thermal contact with a heat reservoir. Now, if the system is immersed in a reservoir such that both heat and particle transports are allowed, then the resulting ensemble is called the *grand canonical ensemble* (GCE). The number fluctuations, in general, are given by Eqs. (2.20) for bosons and (2.21) for fermions. However, the mean occupation number is now different and is given by [1]

$$\langle n_k \rangle = \frac{1}{e^{(\epsilon_k - \mu)\beta} \mp 1}, \tag{2.22}$$

where the $(-)$ and $(+)$ signs correspond to bosons and fermions, respectively. The chemical potential μ is fixed by the requirement that the sum of all $\langle n_j \rangle$ yields the assigned average number of particles $\langle N \rangle$,

$$\langle N \rangle = \sum_k \langle n_k \rangle . \tag{2.23}$$

Note that in the grand canonical treatment, even though the system is allowed to exchange particles with a reservoir, the *average* total number of particles is still fixed. The occupation numbers of the single-particle states fluctuate, both because there are transitions between the states, and also because the system exchanges particles with the reservoir. The mean squared fluctuation of the quantum state k may be obtained from

$$\begin{aligned} \langle \triangle n_k^2 \rangle &= \frac{1}{\beta} \frac{\partial \langle n_k \rangle}{\partial \mu}, \\ &= \frac{e^{(\epsilon_k - \mu)\beta}}{[e^{(\epsilon_k - \mu)\beta} \mp 1]^2}, \\ &= \langle n_k \rangle (1 \ \pm \langle n_k \rangle), \end{aligned} \tag{2.24}$$

where the upper sign is for bosons and the lower fermions. Note that the bosonic ground state fluctuation may now be determined without the need of the second moment:

$$\langle \triangle {N_0}^2 \rangle = \langle n_0 \rangle (1 + \langle n_0 \rangle). \tag{2.25}$$

This formula was earlier quoted in section 1.1, and the corresponding GCE fluctuation catastrophe was also described.

2.2 The Many-Body Quantum Systems

In this section we examine in a more detail the many-body multiplicity of states $\Omega(E_n, N)$ of the energy eigenvalue E_n. This quantity was cited earlier in sections 2.1.1 and 2.1.2. Here, we shall study it more closely, starting from a single-particle energy spectrum. We shall also look at a related quantity called the quantum density of states.

2.2.1 The multiplicity of states

For a given single-particle quantum energy spectrum, the single-particle multiplicity is the degeneracy of the state i with energy ϵ_i. Given N noninteracting particles, or noninteracting quasiparticles in the mean field, the corresponding eigenenergy spectrum is the many-body E_n, and the corresponding quantity of interest is the many-body multiplicity $\Omega(E_n, N)$. In principle this quantity may be found by filling up the N particles in the single-particle energy spectrum ϵ_i, then counting the number of configurations that have the same energy such that

$$E = \sum_{\{N_i\}} N_i \epsilon_i, \tag{2.26}$$

where N_i is the number of particles occupying level i, $\{N_i\}$ denotes all the possible configurations having energy E. The different values of E form a many-body energy spectrum $E_1, E_2, \ldots$. The number of configurations that have the same energy E_n, $n = 1, 2, \ldots$, is the many-body multiplicity of states $\Omega(E_n, N)$. Clearly, this is identical to the degeneracy of the many-body energy level with eigenvalue E_n.

For clarity let us consider an example. For simplicity we take the particles to be bosons. Let the single-particle energy spectrum assume squared integer values in some suitably scaled units, *i.e.*, $\epsilon_m = m^2$, $m = 0, 1, 2, \ldots$. Fig. 2.1a shows the different configurations in which the particles are distributed in increasing excitation energy E, up to $E = 5$. We assume the number of particles N to be large. This is represented by a thick line at $\epsilon_0 = 0$. The lowest state is the one in which all the particles are in the ground state, where $E = 0$, and there is only one configuration for this. Thus $\Omega(0, N) = 1$. For some values of E there is only one configuration that satisfies Eq. (2.26), such as when $E = 1, 2$, and 3. For other values of E, there may be more than one configuration that satisfy the same condition, such as when $E = 4, 5$ and so on. These energies constitute the many-body energy spectrum $E_n = n$, where n is integer, shown in Fig. 2.1b. The corresponding degeneracy for each level is also shown in brackets.

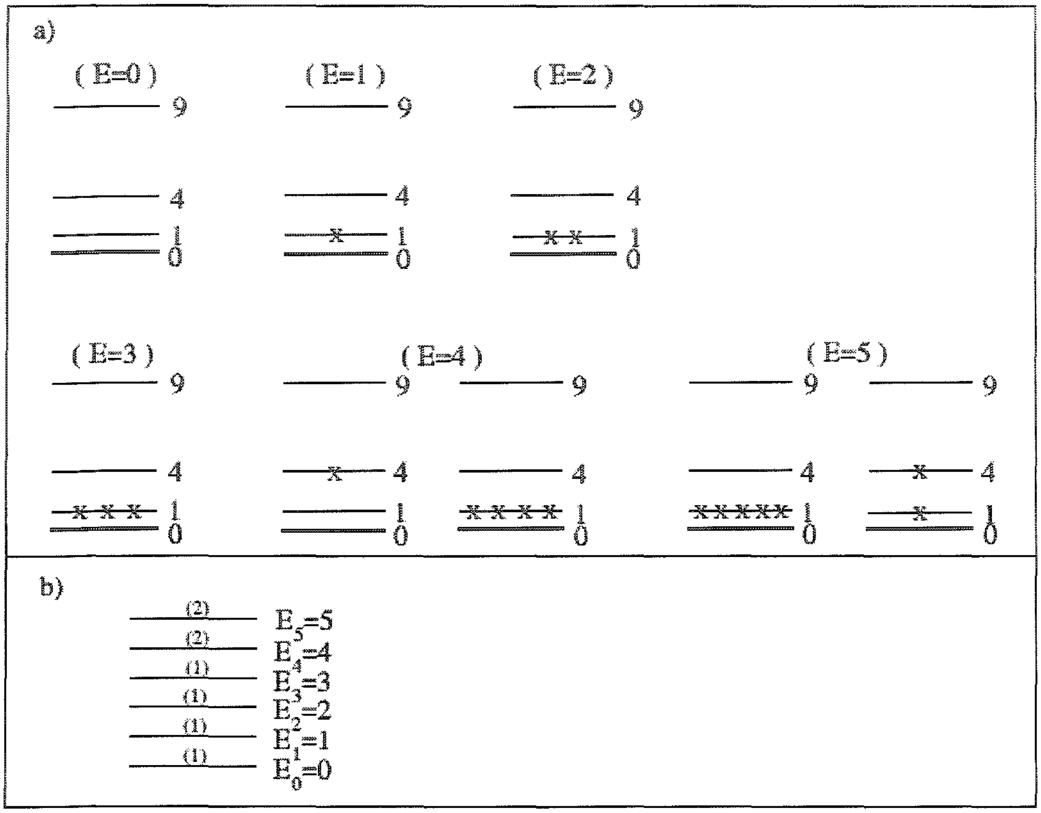


Figure 2.1: a) Example of distributing N particles over the levels of a single-particle energy spectrum, given by $\epsilon_m = m^2$, $m = 1, 2, 3....$ The number of particles are assumed to be large. The higher energy levels are not shown. The total energy E of each configuration is shown in brackets. b) The many-body energy spectrum $E_n = n$, n integer. The corresponding degeneracy for each level is also shown in brackets.

To list, the degeneracies of these many-body energy levels are

$$\Omega(0, N) = 1,$$
$$\Omega(1, N) = 1,$$
$$\Omega(2, N) = 1,$$
$$\Omega(3, N) = 1,$$
$$\Omega(4, N) = 2,$$
$$\Omega(5, N) = 2.$$

The process may be continued on for larger energies. Clearly, the degeneracy $\Omega(E_n, N)$ increases with increasing energies. It may be noted that this calculation is quite tedious, especially for larger energy, and an analytical formula for the multiplicity is much preferred. This formula shall be derived in chapter 3. Note that the single-particle energy spectrum considered in the example is non-degenerate. In general, however, it may not be, and as a result, there would be more combinations of configurations for a given energy E.

Few remarks are in order here. (i) Each configuration shown in Fig. 2.1a is called a microstate $\omega(E, N_{ex}, N)$, where N_{ex} is the number of particles in the excited states. Thus, from the figure,

$$\begin{aligned}
&\omega(0,0,N) = 1, \\
&\omega(1,1,N) = 1, \quad \omega(1, N_{ex} \neq 1, N) = 0, \\
&\omega(2,2,N) = 1, \quad \omega(2, N_{ex} \neq 2, N) = 0, \\
&\omega(3,3,N) = 1, \quad \omega(3, N_{ex} \neq 3, N) = 0, \quad etc.
\end{aligned}$$

Recall in section 2.1.1 the multiplicity $\Omega(E, N)$ is defined as a sum of these microstates for a fixed energy. By summing the microstates above over N_{ex} one gets the multiplicity or the many-body quantum degeneracy $\Omega(E_n, N)$ listed earlier, in accordance with the definition. (ii) The many-body energy spectrum E_n is given by a set of integers, even though the single-particle energy spectrum is not. This is in fact true for any power-law single-particle energy spectrum and noninteracting particles. We shall see that this fact is extremely useful when we look at integer partitioning in chapter 3. (iii) Once the degeneracy $\Omega(E, N)$ are found for a given energy E, then the N-particle partition function may easily be calculated using Eq. (2.13). The exact microcanonical entropy of the N-particle system, denoted by $\mathcal{S}_N(E)$, is uniquely defined as

$$\mathcal{S}_N(E) = \ln \Omega(E, N) \tag{2.27}$$

for a given energy E. We next look at a different quantity, known as the density of states, and establish its relationship with the above quantum degeneracy.

2.2.2 The density of states

The N-particle partition function given by Eq. (2.13) may also be cast in a different form [48]:

$$Z_N = \int_0^\infty \rho_N(E) e^{-\beta E} dE, \tag{2.28}$$

where $\rho_N(E)$ is the quantum *density of states* and is defined as

$$\rho_N(E) = \sum_n \Omega(E_n, N)\delta(E - E_n). \tag{2.29}$$

The density of states may be found by taking the Laplace inverse of Eq. (2.28):

$$\rho_N(E) = \mathcal{L}_\beta^{-1} Z_N = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} Z_N e^{\beta E} d\beta. \tag{2.30}$$

Note that in quantum statistics and thermodynamics β has the physical significance of an inverse temperature, $\beta = 1/T$ (recall we have put the Boltzmann constant k_B to be unity). Here, however, it needs not have that meaning, but is only a mathematical dummy variable. After doing the inverse transform Eq. (2.30), β is no longer present and $\rho_N(E)$ is only a function of the energy E. Let us consider a concrete example. For the N-particle quantum spectrum considered in the example in previous section, the partition function is given by

$$Z_N = 1 + e^{-\beta} + e^{-2\beta} + e^{-3\beta} + 2e^{-4\beta} + 2e^{-5\beta} + 2e^{-6\beta} + 2e^{-7\beta} + 3e^{-8\beta} + \ldots.$$

Taking the Laplace inverse term by term and using

$$\mathcal{L}_\beta^{-1}\left(e^{-a\beta}\right) = \delta(E - a),$$

we see that

$$\begin{aligned} \rho_N(E) &= \mathcal{L}_\beta^{-1} Z_N \\ &= \delta(E) + \delta(E-1) + \delta(E-2) + \delta(E-3) + 2\delta(E-4) + 2\delta(E-5) + 2\delta(E-6) \\ &\quad +2\delta(E-7) + 3\delta(E-8) + \ldots \end{aligned}$$

which clearly has the form given by Eq. (2.29).

One basic feature of the density $\rho_N(E)$ is that it may be decomposed into an averaged smooth part $\bar{\rho}_N(E)$ and an oscillating part $\delta\rho_N(E)$ [48]:

$$\rho_N(E) = \bar{\rho}_N(E) + \delta\rho_N(E). \tag{2.31}$$

To see this, assume the many-body eigenenergies E_n to be given by a function $f(n)$, where $f(n)$ has a differentiable inverse $f^{-1}(x) = F(x)$, such that $n = F(E_n)$. The quantum degeneracy of the states at energy E_n is given by $\Omega(E_n, N)$. Changing variable from E to n in the delta function

$$\delta(E - E_n) = \delta(E - f(n)) = \delta(n - F(E))|F'(E)|,$$

then Eq. (2.29) may be rewritten in as [49]

$$
\begin{aligned}
\rho_N(E) &= \sum_n \Omega(E_n, N)\delta(E - E_n), \\
&= \sum_n \Omega(E_n, N)\delta(n - F(E))|F'(E)|, \\
&= \Omega(E, N)|F'(E)| \sum_n \delta(n - F(E)), \\
&= \Omega(E, N)|F'(E)| \left[1 + 2\sum_{k=1}^{\infty} cos\,(2\pi k F(E))\right]. \qquad (2.32)
\end{aligned}
$$

In the last step of the above we have used the Poisson sum formula

$$
\begin{aligned}
\sum_{n=0}^{\infty} \delta(x - n) &= \sum_{k=-\infty}^{\infty} e^{2\pi i k x} \\
&= 1 + 2\sum_{k=1}^{\infty} cos(2\pi k x), \ E \geq 0.
\end{aligned}
$$

The first term on the RHS of Eq. (2.32) is the smoothly varying part of the density of states $\bar{\rho}_N(E)$, while the second is the oscillating component $\delta\rho_N(E)$. In this work we are mainly interested in the smooth part (see Ref. [48] for the significance of the oscillating part in connection to periodic orbits theory). We then obtain an important relation

$$\bar{\rho}_N(E) = \Omega(E, N)|F'(E)|. \qquad (2.33)$$

Note that when the change of variable $E_n \to E$ is made in $\Omega(E_n, N)$, where E is a continuous variable, the function $\Omega(E, N)$ is now a smooth function of E and N. As mentioned before, this quantity is in general exceedingly difficult to determine. This can be clearly seen even from the simple examples shown in Figs. 1.1 and 2.1. However, if an analytical formula for the smooth part of the density of states $\bar{\rho}_N(E)$ can be found, the quantum degeneracy may be determined using relation (2.33). With the help of the saddle point method, the smooth part may be obtained from Eq. (2.30). The result is (see Appendix B for detail)

$$\bar{\rho}_N(E) = \frac{e^{S_N(\beta_0)}}{\sqrt{2\pi S''_N(\beta_0)}}, \qquad (2.34)$$

where $S_N(\beta_0) = \beta_0 E + \ln Z_N$ is the canonical entropy evaluated at the stationary point β_0.

2.3 The Generating Functions

This section serves to review some background and insight into the number partitioning theory, and introduces the so-called generating function which, as shall be seen, is very useful for our work. The connection between the materials presented here to the number fluctuation shall be made clear in subsequent chapters.

The problem that we are interested in is fundamental in additive number theory. It is that of partitioning an integer n into summands consisting of positive integers or their powers $\leq n$. The summands are called parts, and the order of the parts is irrelevant. We focus the discussion on the case where the parts are positive integers first, and consider the other cases after. As an example, the integer 5 may be partitioned into 1, 2, 3, 4 and 5 parts as follows:

$$\begin{aligned} 5 &= 5, \\ &= 1+4,\ 2+3, \\ &= 1+1+3,\ 1+2+2, \\ &= 1+1+1+2, \\ &= 1+1+1+1+1. \end{aligned} \tag{2.35}$$

In the above example, there is no restriction on the number of parts and the parts are allowed to repeat. The number of ways an integer n can be written as a sum of summands without any restriction on the number of parts and with repetition is known as *unrestricted integer partitioning* and is denoted by $p(n)$. From the example, it can be seen that $p(5) = 7$. The generating function for $p(n)$, due to Euler, is given by [42]

$$f(x) = \prod_{m=1}^{\infty} \frac{1}{1-x^m} = \sum_{n=0}^{\infty} p(n)\ x^n, \tag{2.36}$$

where $|x| < 1$.

If the number of parts (or the size of partitions) is restricted, the problem is then known as *restricted integer partitioning*. We denote this quantity, *i.e.* the number of partitions of n in which at most N parts appear, to be $p_N(n)$. We wish to find the generating function for $p_N(n)$. In number theory there are a number of partition problems which may be solved by using a graphical representation, including the problem that we are interested in. In the graphical representation, a partition is represented by horizontal rows of dots. Consider the integer 5. One partition of 5, given by

$$1+1+1+2,$$

can be represented by 5 dots arranged in 4 rows as follows:

$$\begin{array}{ll} \cdot & \\ \cdot & \\ \cdot & \\ \cdot & \cdot \end{array}$$

Reading this graph vertically from left to right, one gets another partition of 5,

$$4 + 1.$$

Note that the number of parts in the first partition (which is equal to 4) is equal to the *largest* part in the second partition (which is also equal to 4). This brings us to an important theorem in number partitioning theory [50, 51]: if we denote $\pi_N(n)$ to be the number of partitions of n in which each part is no larger than N, then

$$p_N(n) = \pi_N(n). \tag{2.37}$$

In words, Eq. (2.37) states that *the number of partitions of n into at most N parts is equal to that in which each part is no larger than N*. The generating function for $\pi_N(n)$ is known:

$$f_N(x) = \prod_{m=1}^{N} \frac{1}{1 - x^m} = \sum_{n=0}^{\infty} \pi_N(n)\ x^n. \tag{2.38}$$

Since $p_N(n) = \pi_N(n)$, Eq. (2.38) is therefore also the generating function for the number of restricted partitions of n, $p_N(n)$:

$$f_N(x) = \prod_{m=1}^{N} \frac{1}{1 - x^m} = \sum_{n=0}^{\infty} p_N(n)\ x^n. \tag{2.39}$$

So far we have considered unrestricted and restricted partitions in which the parts are allowed to repeat. We shall also consider the cases in which the parts are *distinct*. In general, integer partitioning may fall in one of the following four categories (with the corresponding notation used in brackets):

1)	Unrestricted partitions ($p(n)$):	the number of parts is unrestricted and repetition is allowed;
2)	Unrestricted distinct partitions ($d(n)$):	the number of parts is unrestricted but repetition is not allowed;
3)	Restricted partitions ($p_N(n)$):	the number of parts is restricted and repetition is allowed;
4)	Restricted distinct partitions ($d_N(n)$):	the number of parts is restricted and repetition is not allowed.

In addition to being in one of the four categories described above, an integer n may also be partitioned into parts which are odd, even, primes, squares, cubes,... etc. For our purpose we consider the case in which n is partitioned into sum of s^{th} powers of a set of integers, where $s = 1, 2, 3, \ldots$. We have so far looked at the $s = 1$ case. For other values of s we shall add a superscript (s) to the symbols used in the different partitioning categories. As an example, consider partitioning the integer 5 into sum of squares, *i.e.* $s = 2$. The partitions are

$$1^2 + 2^2, \; 1^2 + 1^2 + 1^2 + 1^2 + 1^2.$$

Thus,

$$p^{(2)}(5) = 2.$$

There is only one way of partitioning 5 into distinct squares, however, since only

$$1^2 + 2^2,$$

is admissible. Thus

$$d^{(2)}(5) = 1.$$

In the case of unrestricted partitions, with repetition or distinct, the generating functions are known for a general s. However, in the restricted case, the only generating function known is for the number of restricted partitions of n, $p_N(n)$ $(s = 1)$. Recall that this is found using the identity (2.37). There is no such relation for other values of s, and the generating functions for these cases are not known. As shall be shown in section 3.4, by using a model consisting of the particle sector of N fermions in a one-dimensional harmonic spectrum, the generating function for the number of restricted distinct partitions of n with $s = 1$ $(d_N(n))$ is determined. In table 2.1 we list the generating functions for the cases just discussed and in the four categories mentioned earlier [50, 52]. Those that are not known are listed as N/A.

		Unrestricted	Restricted
$s=1$	With repetition ($p(n)$ & $p_N(n)$)	$\prod_{m=1}^{\infty}\frac{1}{1-x^m}$	$\prod_{m=1}^{N}\frac{1}{1-x^m}$
	Distinct ($d(n)$ & $d_N(n)$)	$\prod_{m=1}^{\infty}(1+x^m)$	To be found in section 3.4
$s>1$	With repetition ($p^{(s)}(n)$ & $p_N^{(s)}(n)$)	$\prod_{m=1}^{\infty}\frac{1}{1-x^{m^s}}$	N/A
	Distinct ($d^{(s)}(n)$ & $d_N^{(s)}(n)$)	$\prod_{m=1}^{\infty}(1+x^{m^s})$	N/A

Table 2.1: List of the generating functions of the number of partitions of n into sum of powers. The generating functions for the restricted cases with $s>1$ are not known, and are listed as N/A.

Chapter 3

The Quantum Density of States and Partitioning an Integer

"One of these men is Genius to the other;
And so of these. Which is the natural man,
And which the spirit? who deciphers them? "
William Shakespeare, Comedy of Errors, Act5, Scene 1

It is well known that for ideal bosons in a one-dimensional harmonic trap, the problem of counting the number of ways of exciting particles for a given energy E is the same as the number of ways of partitioning an integer n into a sum of other integers. In fact, in the example shown in Fig. 1.1b, each microstate corresponds to a partition of the integer 5 into N_{ex} parts, *i.e.*,

$$\begin{aligned} N_{ex} = 1 \rightarrow 5 &= 5, \\ N_{ex} = 2 \rightarrow 5 &= 1+4,\ 2+3, \\ N_{ex} = 3 \rightarrow 5 &= 1+1+3,\ 1+2+2. \end{aligned}$$

Here, the number of parts ($= N_{ex}$) is restricted by the number of particles $N = 3$, which is known as restricted integer partitioning. Recall in section 2.3 we denote this as $p_N(n)$. Clearly, $p_N(n)$ in number theory is equivalent to the many-body quantum degeneracy $\Omega(E, N)$ discussed in chapter 2, when E is identified with n. Had we chosen N to be very large in the example, with either $N \geq E$ or $N \rightarrow \infty$, the problem would then correspond to unrestricted integer partitioning, which we denoted by $p(n)$. An asymptotic (large n) expression for $p(n)$ is given by the famous Hardy-Ramanujan formula, which was derived using advanced mathematics [42]. Grossmann and Holthaus have made use of this formula to calculate the microcanonical number fluctuation from the ground state of bosons in the one-dimensional harmonic system [9, 10]. In this chapter we use the connection between the many-body quantum degeneracy and the density of states (see section 2.2.2), the latter of which may be derived using the methods in statistical mechanics, to obtain the Hardy-Ramanujan formula as well as those for partitioning of an integer into a sum of squares ($s = 2$), or a sum of cubes ($s = 3$), etc. In general, the problem is equivalent to distributing N bosons over a set of energy levels given by the single-particle power-law spectrum, $\epsilon_m = m^s,\ m = 0, 1, 2 \ldots.$ While the "physicists derivation" of the number partitions has been known for a while and has been extensively used in the analysis of number fluctuation in a one-dimensional harmonically trapped bose gases, the derivation for a general power-law spectrum given above is novel even though the result was derived long ago by Hardy and Ramanujan using more advanced methods. In addition to deriving the asymptotic formulae for the number of partitions of n, both unrestricted and restricted, we also show that by extending the method, we are able to obtain similar formulae for the number of *distinct* partitions. Some of the results pertaining to the partitions of an integer into a sum of distinct powers, to the best of our knowledge, are new, and will be pointed out as they appear in the text.

3.1 The number of partitions of n

In this section we consider a general unrestricted integer partitioning, that of partitioning an integer n into a sum of s^{th} powers of a set of integers. Our purpose is to find an asymptotic formula for $p^{(s)}(n)$. Recall in section 2.2.2, for $s = 1$ this is equivalent to finding $\bar{\rho}(E)$, which is given by

$$\bar{\rho}(E) = \frac{e^{S(\beta_0)}}{\sqrt{2\pi S''(\beta_0)}}, \tag{3.1}$$

and use relation (2.33) to obtain the asymptotic formula for $\Omega(n)$, which is identical to $p(n)$. To simplify the notation, we have excluded the "N" in $\Omega(n)$ and $p(n)$ for unrestricted partition. We shall apply the same technique for general s, and obtain a general formula for unrestricted integer partitioning known in the literature.

The single-particle energy spectrum is given by $\epsilon_m = m^s$, where $m = 0, 1, 2 \ldots$, and $s > 0$ for a system of bosons. The energy is measured in dimensionless units. For example, when $s = 1$ the spectrum can be mapped on to the (shifted) spectrum of a one-dimensional oscillator where the energy is measured in units of $\hbar\omega$. For $s = 2$, it is equivalent to setting energy unit as $\hbar^2/2m$, where m is the particle mass in an infinite one-dimensional square well of unit length. Note that for this case a connection to number partitioning theory is possible only when a fictitious ground state of zero energy is added to the square well spectrum. We have already assumed this in the example given in Fig. 2.1. This is also true for other values of $s \neq 1$. The only two physically interesting cases are $s = 1$, and 2. We however keep s arbitrary even though for $s > 2$ there are no quadratic hamiltonian systems. In particular s needs not even be an integer except to allow a comparison between the number theoretic results for $p^{(s)}(n)$ and the density of states $\bar{\rho}^{(s)}(E)$ that we obtain here. Before we proceed, it is important to note that the many-body eigenenergies are given by a set of integers, $E_n = n$, for a general single-particle power-law energy spectrum (see section 2.2.1, in particular the example shown in Fig. 2.1 where the single-particle energy spectrum is given by a set of squares). This implies that the factor $|F'(E)|$ in Eq. (2.33) is unity:

$$|F'(E)| = 1.$$

Thus, in general for a single-particle power-law spectrum,

$$p(n) \sim \bar{\rho}(E),$$

$$p_N(n) \sim \bar{\rho}_N(E),$$

where the symbol "$\sim$" means "asymptotically equals".

The many-body partition function for N noninteracting bosons in a single-particle power-law spectrum, with $N \to \infty$, is given by the generating function for the number of unrestricted partitions of an integer n into sum of s^{th} powers of a set of integers. From section 2.3, table 2.1, this is given by

$$\begin{aligned} Z(\beta) &= \sum_n \Omega(E_n) e^{-\beta E_n}, \\ &= \sum_{n=1}^{\infty} p^{(s)}(n) x^n, \\ &= \prod_{m=1}^{\infty} \frac{1}{[1-\exp(-\beta m^s)]}, \end{aligned} \tag{3.2}$$

where we have identified $x = e^{-\beta}$, and made explicit that Z is a function of β. We now proceed to calculate the asymptotic formula for $p^{(s)}(n)$ using Eq. (3.1). The entropy is given by

$$\begin{aligned} S(\beta) &= \beta E + \ln Z(\beta), \\ &= \beta E - \sum_{j=1}^{\infty} \ln\left(1 - e^{-\beta j^s}\right). \end{aligned} \tag{3.3}$$

Using Euler-Maclaurin summation formula [1],

$$\begin{aligned} \ln Z(\beta) &= -\sum_{j=1}^{\infty} \ln\left(1 - e^{-\beta j^s}\right), \\ &= \int_0^{\infty} \ln\left(1 - e^{-\beta j^s}\right) dj + \frac{1}{2}\ln\beta - \frac{s}{2}\ln 2\pi + O(\beta), \\ &= \frac{1}{\beta^{1/s}}\Gamma(1+1/s)\zeta(1+1/s) - \frac{s}{2}\ln 2\pi + O(\beta), \end{aligned}$$

where $\Gamma(x)$ is the Gamma function and the zeta function $\zeta(x)$ is defined as

$$\zeta(x) = \sum_{j=1}^{\infty} \frac{1}{j^x}. \tag{3.4}$$

Defining

$$C(s) = \Gamma(1+\frac{1}{s})\zeta(1+1/s),$$

the entropy becomes

$$S(\beta) = \beta E + \frac{C(s)}{\beta^{1/s}} + \frac{1}{2}\ln\beta - \frac{s}{2}\ln(2\pi) + O(\beta). \tag{3.5}$$

Assuming small β (large E), we neglect terms of order β or higher. Further, for determining the stationary point, we ignore the $\ln\beta$ term in the derivative of S. Thus in the leading order,

$$S'(\beta) = E - \frac{1}{s}\,\frac{C(s)}{\beta^{(1+1/s)}}\,. \tag{3.6}$$

The saddle point is found by setting the above to be zero and is given by

$$\beta_0 = \left(\frac{C(s)}{sE}\right)^{s/(1+s)}. \tag{3.7}$$

The notation may be simplified by setting

$$\kappa_s = \left(\frac{C(s)}{s}\right)^{\frac{s}{1+s}},$$

[1]It is easier to use mathematical computer program for this, such as Maple, the syntax of which is: readlib(eulermac), eulermac(f(n),n=a..b) where a and b are the upper and lower summation limits.

so that

$$\beta_0 = \kappa_s \, E^{-\frac{s}{1+s}}. \tag{3.8}$$

The entropy, evaluated at the saddle point, is

$$S(\beta_0) = (1+s)\kappa_s E^{1/(1+s)} + \frac{1}{2}\ln\kappa_s - \frac{s}{2(1+s)}\ln E - \frac{s}{2}\ln 2\pi. \tag{3.9}$$

Next, the second derivative, evaluated at the saddle point, is

$$\begin{aligned} S''(\beta_0) &= \frac{1+s}{s}\frac{C(s)}{s}\left(\frac{s}{C(s)}E\right)^{\frac{1+2s}{1+s}}, \\ &= \frac{1+s}{s}\frac{E^{\frac{1+2s}{1+s}}}{\kappa_s}. \end{aligned} \tag{3.10}$$

Substituting Eqs. (3.9) and (3.10) in the saddle point expression for the density of states Eq. (3.1) and simplifying, we obtain

$$\overline{\rho}^{(s)}(E) = \frac{\kappa_s}{(2\pi)^{\frac{(s+1)}{2}}}\sqrt{\frac{s}{s+1}}E^{-\frac{3s+1}{2(s+1)}}\exp\left[\kappa_s(s+1)E^{\frac{1}{1+s}}\right]. \tag{3.11}$$

The above equation is identical to that given for $p^{(s)}(n)$ in Ref. [42], the number of ways of expressing n as a sum of integers with s^{th} powers, if we replace E by the integer n. For $s=1$, for example, we have

$$\overline{\rho}(E) = \frac{\exp[\pi\sqrt{\frac{2E}{3}}]}{4\sqrt{3}E}, \tag{3.12}$$

which is the well known Hardy-Ramanujan formula. For $s=2$, the asymptotic density of states is

$$\overline{\rho}^{(2)}(E) = \sqrt{\frac{2}{3}}\frac{\kappa_2}{(2\pi)^{3/2}}\frac{\exp[3\kappa_2 E^{1/3}]}{E^{7/6}}, \tag{3.13}$$

with $\kappa_2 \approx 1.10247$. This is the same as the asymptotic formula derived by Hardy and Ramanujan for the number of partitions of E into squares. It is to be noted that in making the identification of $p^{(2)}(n)$ with $\overline{\rho}^{(2)}(E)$, $E=n$ is to be identified as the excitation energy of the quantum system with a fictitious ground state at zero energy added to the square well.

In Fig. 3.1 we show a comparison between the exact (computed) $p(n)$ (solid line), and $\overline{\rho}(E)$ (dashed line), as given by Eq. (3.12). We note that the Hardy-Ramanujan formula works well even for small n. Similarly, in Fig. 3.2, the computed $p^{(2)}(n)$ is compared with $\overline{\rho}^{(2)}(E)$, as given by Eq. (3.13). The comparison for $s=3$ is made in Fig. 3.3. In all these figures the computed partitions $p^{(s)}(n)$ have step-like discontinuities, unlike the smooth behavior of $\overline{\rho}^{(s)}(E)$, specially for small n (or E).

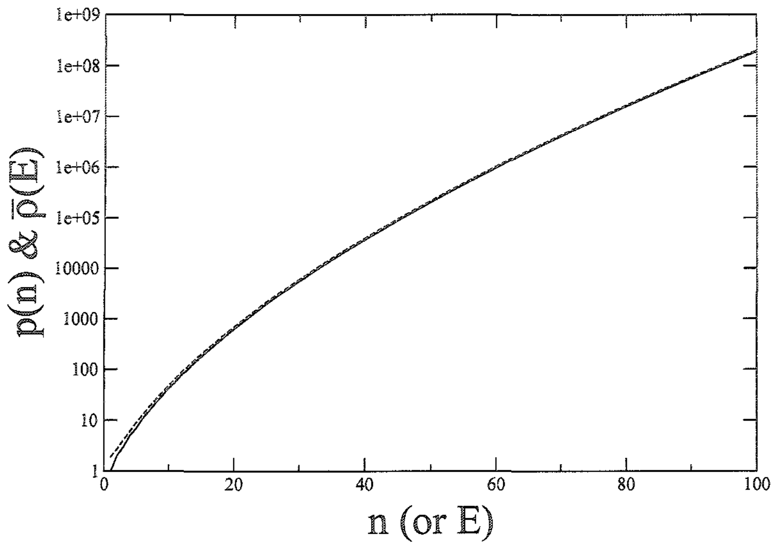


Figure 3.1: Comparison of the exact $p(n)$ (solid line) and the asymptotic $\overline{\rho}(E)$ (dashed line), obtained from Eq. (3.12) for $s = 1$.

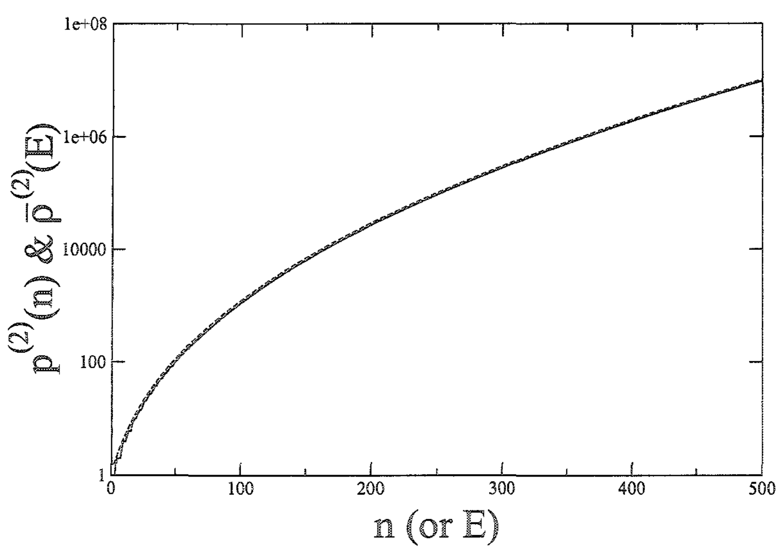


Figure 3.2: Comparison of the exact $p^{(2)}(n)$ (solid line) and the asymptotic $\overline{\rho}^{(2)}(E)$ (dashed line), obtained from Eq. (3.13) for $s = 2$.

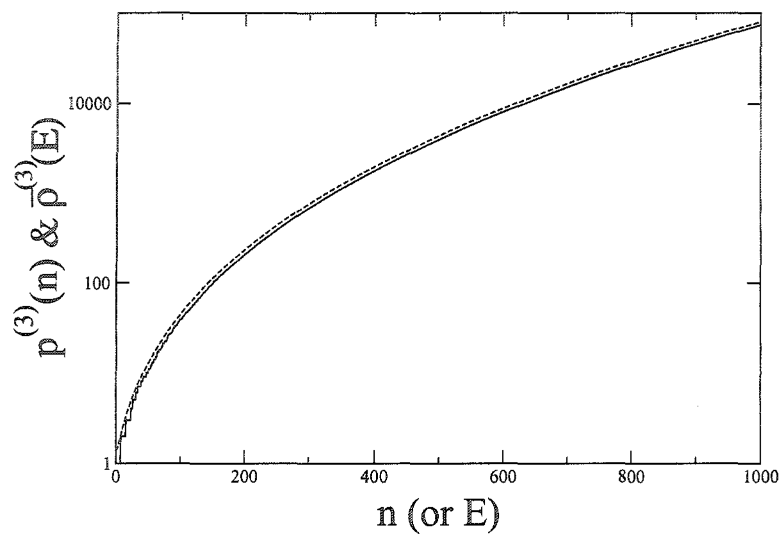


Figure 3.3: Same as Figs. 3.1 and 3.2, except $s = 3$. The asymptotic $\overline{\rho}^{(3)}(E)$ is obtained from Eq. (3.11) with $s = 3$.

3.2 The number of restricted partitions of n

We now apply the same method to obtain the asymptotic density of states for systems with finite size, that is when the number of particles is kept finite and equal to N. This corresponds to allowing the number of parts to be at most N, *i.e.*, restricted integer partitioning. However, we restrict to the $s = 1$ case only, since the restricted partition functions for other s are not known.

Our quantum mechanical system is a system consisting of N bosons in a one-dimensional harmonic oscillator, where N is finite. Our purpose is to calculate the asymptotic density of states of this system. The many-body partition function in this case is given by the generating function for the number of restricted partitions of an integer n into a sum of other integers $\leq n$. From section 2.3, Eq. (2.39) or table 2.1, this is given by

$$\begin{aligned} Z_N(\beta) &= \sum_n \Omega(E_n, N) e^{-\beta E_n}, \\ &= \sum_{n=1}^{\infty} p_N(n) x^n, \\ &= \prod_{m=1}^{N} \frac{1}{[1-\exp(-\beta m^s)]}. \end{aligned} \tag{3.14}$$

Henceforth we shall use the condition of large N and E such that

$$\begin{aligned} N \gg 1, \ \exp(-\beta N) &\ll 1, \\ \beta &\ll 1. \end{aligned} \tag{3.15}$$

Again using Euler-Maclaurin summation formula,

$$\begin{aligned} \ln Z_N(\beta) &= -\sum_{j=1}^{N} \ln\left(1 - e^{-\beta j^s}\right), \\ &\approx \frac{\pi^2}{6\beta} - \frac{1}{\beta}\sum_{j=1}^{\infty}\frac{e^{-jN\beta}}{j^2} + \frac{1}{2}\ln\beta - \frac{1}{2}\ln 2\pi + \frac{1}{2}\sum_{j=1}^{\infty}\frac{e^{-jN\beta}}{j} - \frac{1}{24}\beta. \end{aligned}$$

Next, we need to compare all the terms in the above. To do this we choose $N = 1000$ and $\beta = 1/98$ (note that these values satisfy condition 3.15), then

1^{st} term	$\rightarrow$	$\frac{\pi^2}{6\beta}$	$\approx$	161.2,
2^{nd} term	$\rightarrow$	$\frac{1}{\beta}\sum_{j=1}^{\infty}\frac{e^{-jN\beta}}{j^2}$	$\approx$	$3.6 \times 10^{-3} + 3.4 \times 10^{-8} + \ldots,$
3^{rd} term	$\rightarrow$	$\frac{1}{2}\ln\beta$	$\approx$	-2.3,
4^{th} term	$\rightarrow$	$\frac{1}{2}\ln 2\pi$	$\approx$	0.9,
5^{th} term	$\rightarrow$	$\frac{1}{2}\sum_{j=1}^{\infty}\frac{e^{-jN\beta}}{j}$	$\approx$	$1.8 \times 10^{-5} + 3.4 \times 10^{-10} + \ldots,$
6^{th} term	$\rightarrow$	$\frac{1}{24}\beta$	$\approx$	4.3×10^{-4}.

Thus, ignoring terms of order 10^{-3} or higher, we have in leading order

$$\ln Z_N(\beta) = \frac{\pi^2}{6\beta} + \frac{1}{2}\ln\beta - \frac{1}{2}\ln 2\pi - \frac{1}{\beta}e^{-N\beta}.$$

The entropy for finite N is thus

$$
\begin{aligned}
S_N(\beta) &= \beta E + \ln Z_N(\beta), \\
&= \beta E - \sum_{j=1}^{N} \ln\left(1 - e^{-\beta j}\right), \\
&= \beta E + \frac{\pi^2}{6\beta} + \frac{1}{2}\ln\beta - \frac{1}{2}\ln 2\pi - \frac{1}{\beta}e^{-N\beta}.
\end{aligned} \tag{3.16}
$$

To leading order, the first derivative of the N-particle entropy is

$$S'_N(\beta) = E - \frac{\pi^2}{6\beta^2}, \tag{3.17}$$

and the saddle point is

$$\beta_0 = \frac{\pi}{\sqrt{6E}}, \tag{3.18}$$

which may be obtained from Eq. (3.7) with $s = 1$. The entropy and its second derivative evaluated at the saddle point are given by

$$S_N(\beta_0) = \pi\sqrt{2E/3} + \frac{1}{2}\ln\left(\frac{\pi}{\sqrt{6E}}\right) - \frac{1}{2}\ln 2\pi - \frac{\sqrt{6E}}{\pi}e^{-N\frac{\pi}{\sqrt{6E}}}, \tag{3.19}$$

$$S''_N(\beta_0) = \frac{(6E)^{3/2}}{3\pi}. \tag{3.20}$$

Thus, the density of states for finite N is given by

$$\bar{\rho}_N(E) = \frac{1}{4\sqrt{3}E}\exp\left(\pi\sqrt{2E/3} - \frac{1}{\pi}\sqrt{6E}e^{-N\frac{\pi}{\sqrt{6E}}}\right). \tag{3.21}$$

The above expression reproduces the well known correction to the unrestricted partitions due to the restriction on the size of parts (see Erdos and Lehner [43]). With the condition (3.15), we see that Eq. (3.21) is valid in the region

$$\frac{\pi^2}{6} \ll E \ll \frac{\pi^2}{6}N^2.$$

In Fig. 3.4 we compare the two differences, $[\overline{\rho}(E) - p_N(n)]$ (dotted line), and $[\overline{\rho}_N(E) - p_N(n)]$ (solid line) for $N = 20$ (Fig. 3.4a), and $N = 30$ (Fig. 3.4b). In the above, $\overline{\rho}(E)$ is Hardy-Ramanujan formula for the unrestricted integer partitioning and is obtained from Eq. (3.12), $\overline{\rho}_N(E)$ is the Erdos-Lehner formula for the restricted integer partitioning as given by Eq. (3.21), and $p_N(n)$ is the exact (computed) number of restricted partitions of n. Clearly, the former is much larger than the latter, indicating that Eq. (3.21) gives a better approximation to $p_N(n)$.

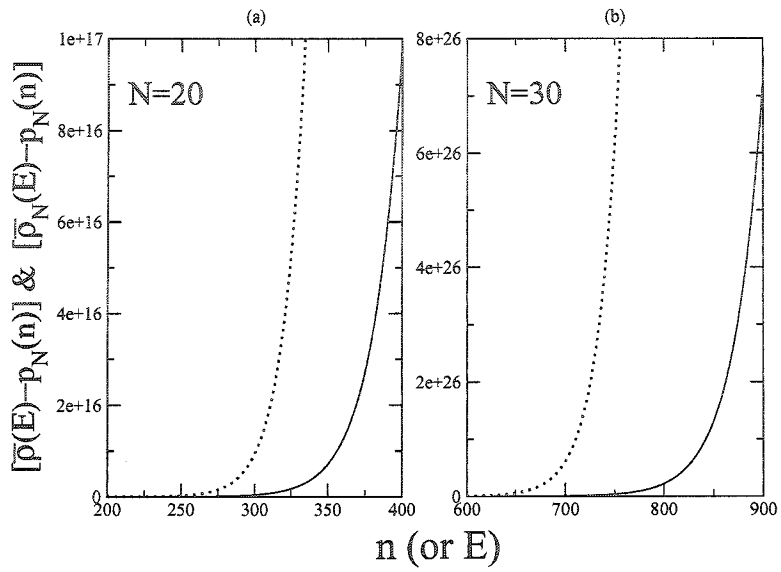


Figure 3.4: (a) Comparison of $[\overline{\rho}(E) - p_{20}(n)]$ (dotted line) and $[\overline{\rho}_{20}(E) - p_{20}(n)]$ (solid line) for $N = 20$, where $\overline{\rho}(E)$ is obtained from Eq. (3.12), $\overline{\rho}_{20}(E)$ is the Erdos and Lehner formula as given by Eq. (3.21), and $p_{20}(n)$ is the exact (computed) restricted partitions. (b) Same for $N = 30$.

3.3 The number of distinct partitions of n

We now modify the method to obtain an asymptotic formula for the number of distinct partitions of an integer n into s^{th} powers, denoted by $d^{(s)}(n)$. For example, for $s = 1$, $n = 5$, the number of distinct integer partitions are 5, 2+3, and 1+4, so $d(5) = 3$. For distinct partitions, one might tempt to draw a parallel with the bosonic case, and reason that this is equivalent to distributing N (spinless) fermions over the energy levels of the single-particle power-law spectrum since the distinctiveness of the parts is immediately ensured by the Pauli principle. However, this is not quite so. Consider the $s = 1$ spectrum and with finite N. The fermionic partition function is given by (setting $x = \exp(-\beta)$ and $E_n = n$ as before),

$$
\begin{aligned}
Z_N(\beta) &= x^{N^2/2} \sum_n \Omega(n, N) x^n, \\
&= x^{N^2/2} \prod_{m=1}^{N} \frac{1}{[1 - x^m]}, \qquad (3.22)
\end{aligned}
$$

which is the same as the bosonic partition function in a harmonic potential, except for the prefactor which is related to the ground state energy of N fermions in the trap. Obviously, the $\Omega(n, N)$ is the same for both fermions and bosons even though $d_N(n)$ is different from $p_N(n)$. This is because the quantum mechanical ground state of fermions consists of occupied levels up to the fermi energy, unlike the bosons which all occupy one single lowest energy state. Clearly, to make a connection to the distinct number partition, one should imagine distributing the N fermions *from the fermi level* (particle space) and disregard the levels below (hole space). The separation of the fermionic levels into 2 separate spaces has been discussed in Ref. [30] in a different context and will be detailed in section 4.1. For the present time, we imagine a system of "pseudo fermions" in which a large number of fermions are put in the Fermi level E_F. They are to be distributed over excited levels according to Pauli principle. The partition function of the particle space, for $N \to \infty$ and general s, is now given by the generating function for the number of unrestricted partitions of an integer n into sums of s^{th} powers of a set of distinct integers. From section 2.3, table 2.1, this is given by

$$\begin{aligned} Z(\beta) &= \sum_{n=1}^{\infty} d^{(s)}(n) x^n, \\ &= \prod_{m=1}^{\infty} \left(1 + \exp(-\beta m^s)\right). \end{aligned} \tag{3.23}$$

We next proceed as before. To leading order the entropy is

$$S(\beta) = \beta E + \frac{D(s)}{\beta^{1/s}} - \frac{1}{2}\ln 2, \tag{3.24}$$

where

$$D(s) = \Gamma(1 + \frac{1}{s})\eta(1 + 1/s).$$

In the above, $\eta(s) = \sum_{l=1}^{\infty} \frac{(-1)^{l-1}}{l^s}$ denotes the alternating zeta function. Note that there is no $\ln(\beta)$ term in Eq. (3.24). The saddle point β_0 is obtained by setting $S'(\beta) = 0$ as before. Defining

$$\lambda_s = (D(s)/s)^{s/(s+1)},$$

the saddle point is given by

$$\beta_0 = \left(\frac{D(s)}{sE}\right)^{s/(1+s)} = \lambda_s \, E^{-\frac{s}{1+s}}. \tag{3.25}$$

The entropy and its second derivative, evaluated at the saddle point, are thus given by

$$S(\beta_0) = (1+s)\lambda_s E^{1/(1+s)} - \frac{1}{2}\ln 2\pi, \tag{3.26}$$

$$S''(\beta_0) = \frac{1+s}{s}\frac{E^{\frac{1+2s}{1+s}}}{\lambda_s}. \tag{3.27}$$

After some tedious algebraic manipulations, the asymptotic expression for the number of unrestricted distinct partitions of an integer $E = n$ is given by

$$\overline{\rho}_F^{(s)}(E) = \sqrt{s\lambda_s}\,\frac{exp\left[(1+s)\lambda_s E^{\frac{1}{1+s}}\right]}{2\sqrt{\pi(1+s)E^{\frac{2s+1}{s+1}}}}, \tag{3.28}$$

where the subscript F in the above formula is to emphasize that Fermi statistics has been used (taking into account only particle space). Once again for $s = 1$ we recover the well known asymptotic formula for the number of unrestricted but distinct partitions $d(n)$ of an integer [53], namely

$$\overline{\rho}_F(E) = \frac{\exp[\pi\sqrt{\frac{E}{3}}]}{4\times 3^{1/4}E^{3/4}}, \tag{3.29}$$

where, as usual, E should be read as n. Similarly the asymptotic expression for $d^{(s)}(n)$ is given by Eq. (3.28). Though the asymptotic expression for $p^{(s)}(n)$ is known, we have not found the general asymptotic expression for $d^{(s)}(n)$ in the literature. This is quite astonishing since the theory of number partition is an old problem, dated back from the time of Euler.

In Fig. 3.5, we show a comparison of the asymptotic density $\overline{\rho}_F(E)$ and the exact distinct partitions $d(n)$ of integer n for $s = 1$. As in the case of bosonic partitions $p(n)$, the asymptotic formula for $d(n)$ works reasonably, except for $n < 10$. Fig. 3.6 shows similar comparison between the exact computations of $d^{(2)}(n)$ and Eq. (3.28) (with $s = 2$). Due to more restrictions in partitioning, the magnitude of $d^{(2)}(n)$ is smaller than that of $d(n)$, and the fluctuations of the data points are more prominent. Despite this, the asymptotic density of states seems to produce a reasonable average of the exact $d^{(2)}(n)$. The absolute ratio of the amplitude of the oscillations to its smooth average value, defined as $R = |d^{(2)}(n) - \rho_F^{(2)}(E)|/\rho_F^{(2)}(E)$, decreases from about 1.5 to 0.2 as n is increased to 1000, as shown in Fig. 3.7. This means that for $n \to \infty$, the smooth part will eventually mask the fluctuations. Fig. 3.8 shows the same comparison for $s = 3$. Here, there are now even more restrictions since the integer is partitioned into distinct cubes.

As a result, the magnitude of $d^{(3)}(n)$ is much smaller than the others, and the fluctuation is now much more pronounced. Similar to the $s = 2$ case, the asymptotic density of states produces a reasonable average of the exact $d^{(3)}(n)$. Due to more fluctuation, the ratio R decreases much more slowly for this case as compared to the $s = 2$ case.

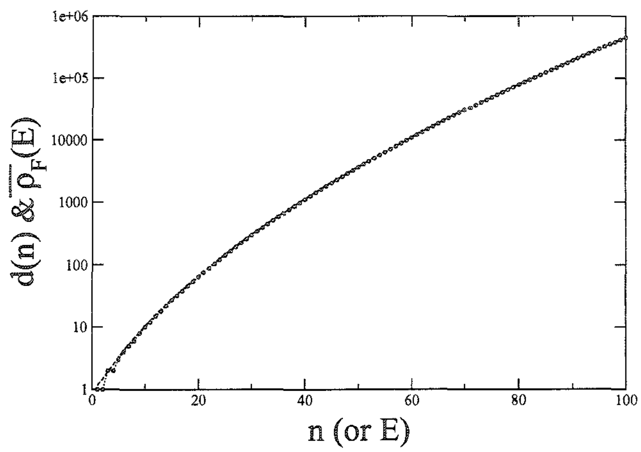


Figure 3.5: Comparison of the exact $d(n)$ (symbol with dotted line) and the asymptotic $\overline{\rho}_F(E)$ (dashed line), obtained from Eq. (3.29) for $s = 1$ and distinct partitions.

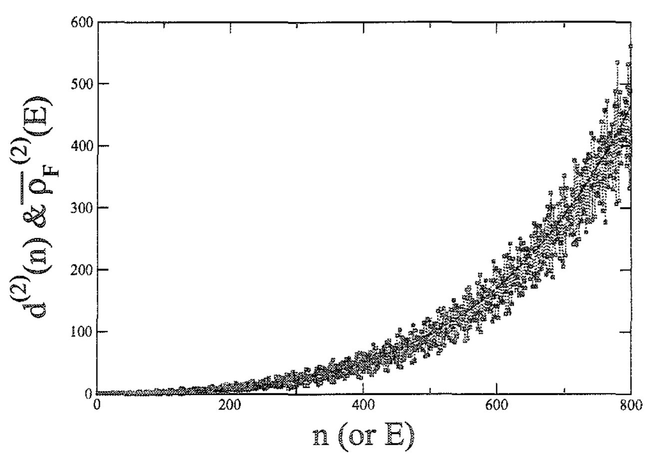


Figure 3.6: Comparison of the exact $d^{(2)}(n)$ (symbol with dotted line) and the asymptotic $\overline{\rho}_F^{(2)}(E)$ (dashed line), obtained from Eq. (3.28) for $s = 2$ and distinct partitions. Note that the y-axis is no longer in log scale.

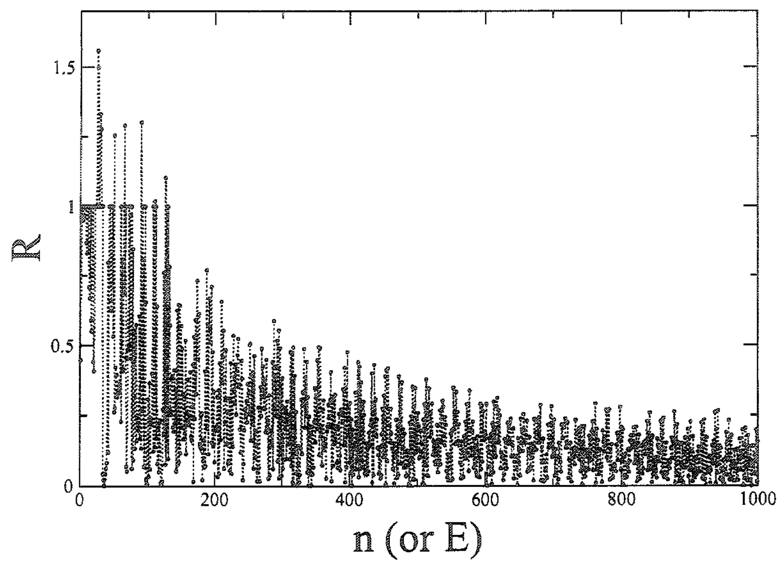


Figure 3.7: Plot of the absolute ratio of the amplitude of the oscillations of $d^{(2)}(n)$ to its average value $\rho_F^{(2)}(E)$, defined as $R = |d^{(2)}(n) - \rho_F^{(2)}(E)|/\rho_F^{(2)}(E)$. The ratio R decreases from about 1.5 to 0.2 as n (or E) increases to 1000.

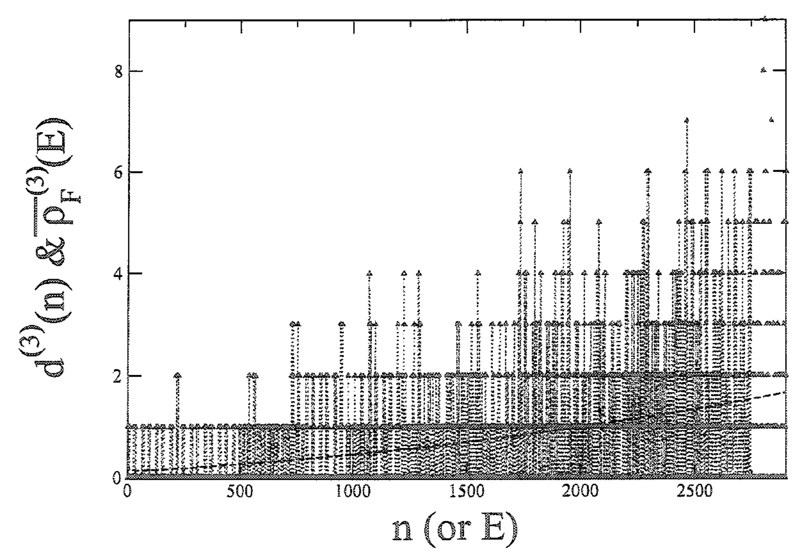


Figure 3.8: Same as Fig. 3.6, except for $s = 3$.

3.4 The number of restricted distinct partitions of n

In the last section of this chapter, we present the finding of an equivalent asymptotic formula to Eq. (3.21) for the number of restricted and distinct partitions of n. What we need is the partition function for the particle space for finite N. One might speculate that in parallel to the finite N bosonic case where repetition of the parts is allowed, the partition function for this distinct case would be Eq. (3.23) with "N" replacing "∞" in the upper limit of the product. However this is incorrect. The reason for it to work in the bosonic case is due to the identity (2.37), discussed in section 2.3. There is no such identity for the distinct case. Fortunately, there is a different theorem known in number theory which we may appeal to [51] (also see Ref. [30] and section 4.1.2): if we denote $\omega^d(n,i)$ to be the number of partitions of n into *exactly* i *distinct* parts, then

$$\omega^d(n,i) = p_i(n - \frac{i(i+1)}{2}), \tag{3.30}$$

where, as before, $p_i(n)$ is the number of partitions of n into parts $\leq$ i. Therefore, the (restricted) number of partitions of n into at most N distinct parts $d_N(n)$ is

$$\begin{aligned} d_N(n) &= \sum_{i=1}^{N} \omega^d(n,i), \\ &= \sum_{i=1}^{N} p_i(n - \frac{i(i+1)}{2}). \end{aligned} \tag{3.31}$$

The generating function for $p_i(n)$ is known and is given by Eq. (3.14). Relation (3.31) implies that the N-particle partition function for the particle space, or equivalently, the generating function for the number of restricted and distinct partitions $d_N(n)$ is given by

$$\begin{aligned} Z_N(\beta) &= \sum_{n=1}^{\infty} d_N(n) x^n, \\ &= \sum_{i=1}^{N} x^{i(i+1)/2} \prod_{n=1}^{i} \frac{1}{(1-x^n)}, \\ &= \prod_{n=1}^{\infty}(1+x^n) - \sum_{i=N+1}^{\infty} x^{i(i+1)/2} \prod_{n=1}^{i} \frac{1}{(1-x^n)}. \end{aligned} \tag{3.32}$$

The first term on the RHS of Eq. (3.32) is the generating function for the number of unrestricted distinct partitions Eq. (3.23) with $s = 1$, and the second term is a sum of the generating functions for the number of restricted partitions Eq. (3.14) with the integer shifted by $i(i+1)/2$. To find an asymptotic formula for the number of restricted distinct partitions $d_N(n)$, as usual, we take inverse Laplace transform of Eq. (3.32). Defining $\triangle_i \equiv i(i+1)/2$, we have:

$$\begin{aligned} d_N(n) &= \mathcal{L}_\beta^{-1}\left\{\prod_{n=1}^{\infty}(1+x^n)\right\} - \sum_{i=N+1}^{\infty}\mathcal{L}_\beta^{-1}\left\{x^{\triangle_i}\prod_{n=1}^{i}\frac{1}{(1-x^n)}\right\}, \\ &= d(n) - \sum_{i=N+1}^{\infty} p_i(n-\triangle_i), \\ &\sim \overline{\rho}_F(E) - \sum_{i=N+1}^{\infty}\overline{\rho}_i(E-\triangle_i). \end{aligned}$$

The formulae for the unrestricted and distinct partitions $\overline{\rho}_F(E)$ and the restricted partition $\overline{\rho}_i(E)$ have already been derived and are given by Eqs. (3.29) and (3.21). Thus,

$$\begin{aligned} d_N(n) &\sim \frac{\exp[\pi\sqrt{\frac{E}{3}}]}{4\times 3^{1/4}E^{3/4}} - \\ &\quad \sum_{i=N+1}^{\infty}\frac{1}{4\sqrt{3}(E-\triangle_i)}\exp\left(\pi\sqrt{\frac{2(E-\triangle_i)}{3}} - \frac{1}{\pi}\sqrt{6(E-\triangle_i)}e^{-N\frac{\pi}{\sqrt{6(E-\triangle_i)}}}\right), \\ &= \overline{\rho}_{N,F}(E). \end{aligned} \tag{3.33}$$

The above is the asymptotic formula for the number of restricted and distinct partitions of an integer n when E is identified with n. Note that $\overline{\rho}_N(E)$ is valid only for $\pi^2/6 \ll E \ll \pi^2/6N^2$, Eq. (3.33) is thus valid only in this range. In Fig. 3.9 we display the two differences, $[\overline{\rho}_F(E) - d_N(n)]$ (dotted line), and $[\overline{\rho}_{N,F}(E) - d_N(n)]$ (solid line) for $N = 20$ (Fig. 3.9a), and $N = 30$ (Fig. 3.9b). In the above differences, $\overline{\rho}_F(E)$ is obtained from Eq. (3.29), $\overline{\rho}_{N,F}(E)$ from Eq. (3.33), and $d_N(n)$ is the exact (computed) number of restricted distinct partitions. Again, similar to the case where repetition of the parts is allowed (Fig. 3.4), the N-correction asymptotic formula gives a better approximation to the exact finite N partition than the infinite one.

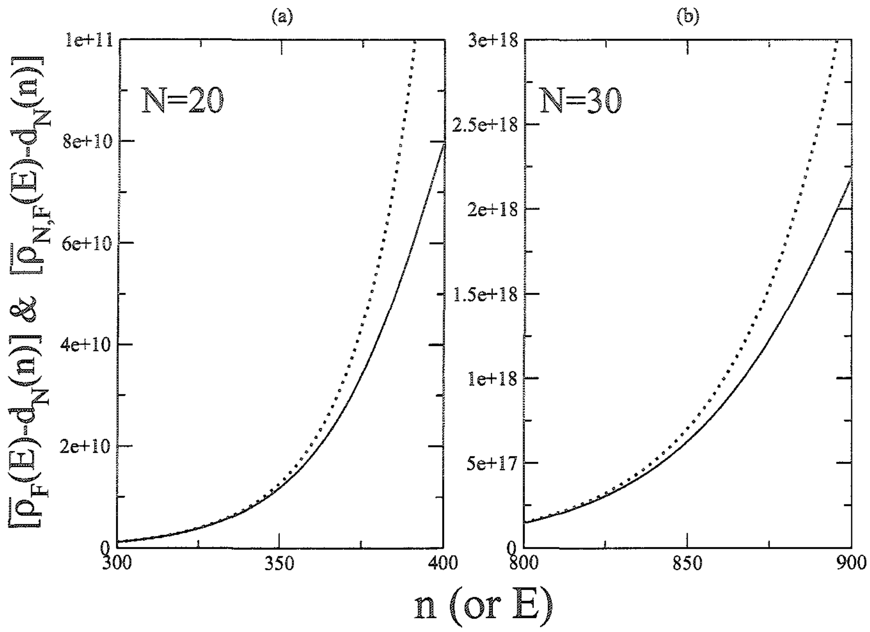


Figure 3.9: (a) Comparison of $[\overline{\rho}_F(E) - d_{20}(n)]$ (dotted line) and $\left[\overline{\rho}_{20,F}(E) - d_{20}(n)\right]$ (solid line) for $N = 20$, where $\overline{\rho}_F(E)$ is obtained from Eq. (3.29), $\overline{\rho}_{20,F}(E)$ from Eq. (3.33), and $d_{20}(n)$ is the exact (computed) number of restricted distinct partitions. (b) Same for $N = 30$.

Before concluding this chapter, it is important to stress again that many results derived here are known in the mathematical literature. However, the general formula for $d^{(s)}(n)$ (Eq. 3.28) and the formula for the number of restricted distinct partitions (Eq. 3.33) are, to the best of our knowledge, new. We emphasize again that we have not found these expressions in the literature. If they are indeed new result, then it is quite surprising that they have not been discovered before, since the theory of partitions has been extensively studied and developed since founded by Euler. The work in this chapter has been reported in Ref. [54].

To conclude this chapter, we show a graph of the exact (computed) multiplicities or the numbers of partitions of n for the different cases discussed here and for $N \to \infty$. Note that the more restriction there is (distinct and/or larger value of s), the less the number of partitions.

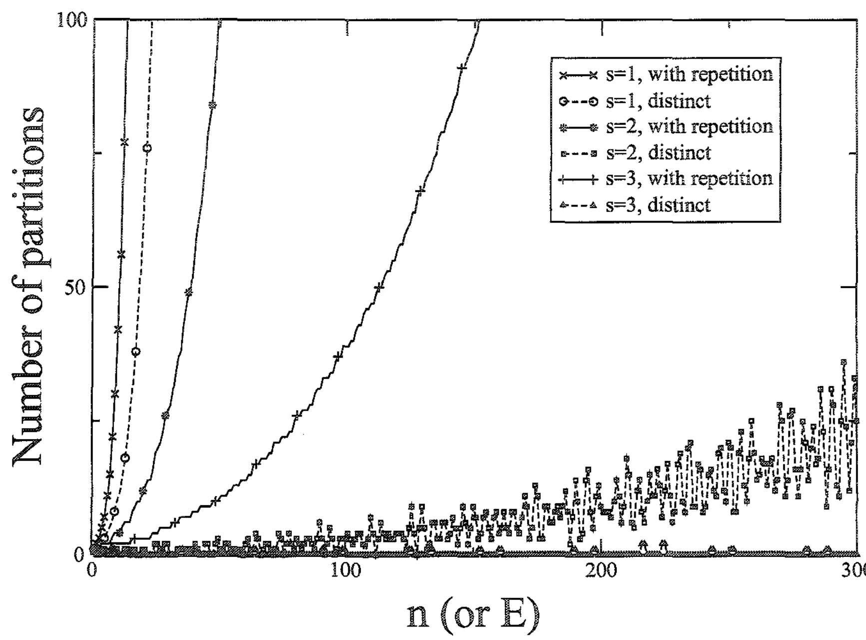


Figure 3.10: Comparison of the different numbers of partitions. The smallest curve, which almost lies on the x axis, corresponds to the one with the most restriction, *i.e.*, $s = 3$ and distinct.

Chapter 4

Number Fluctuation of Noninteracting Trapped Particles

"Symmetry, as wide or as narrow as you may define it, is one idea by which man through the ages has tried to comprehend order, beauty, and perfection."
Hermann Weyl (1885 - 1955)

4.1 Ideal Gas in a one-dimensional Harmonic Trap

The problem of an ideal gas in a one-dimensional harmonic trap has served as a paradigm for many interesting theoretical investigations. Ever since the the observation of BEC in magnetically trapped dilute atomic gasses [6, 7, 8], there had been considerable interest in calculating the ground state number fluctuation of a bose gas in a trap outside the framework of the GCE (see also chapter 1). The one-dimensional harmonic potential is one system that can be treated analytically. Using a number partitioning theory-based approach, a simple expression for the microcanonical number fluctuation as a function of temperature T was derived [9, 15]. In [25, 26], we formulated a combinatorial method for calculating the exact microcanonical number fluctuation from the ground state as a function of excitation energy for both bosons and fermions. Although for fermions there is no grand canonical catastrophe (see chapter 5 for more discussion on this), the work was inspired by the experimental observation of quantum degeneracy in trapped fermionic gas at low temperatures [27, 28]. Even before the experimental work, several theoretical papers had studied the properties of a trapped dilute gas of fermionic atoms. Butts and Rokhsar [55] studied the momentum and spatial distribution of the noninteracting system in the

Thomas-Fermi approximation. Schneider and Wallis [56] looked into other thermodynamic properties of such a gas and the effect of shell structure on the specific heat. The effect of an attractive interaction on the low temperature properties of a trapped fermi gas was investigated by Bruun and Burnett [57]. The collective excitations of the system in the normal phase have been examined by Bruun and Clark [58] and in the superfluid phase by Baranov and Petrov [59]. Recently, resonance condensation of fermionic atom pairs has been experimentally observed [60].

The combinatorics method is, however, very time-consuming computationally. In the case of an ideal boson gas in a one-dimensional harmonic trap, the problem is greatly simplified due to its connection to number partitioning theory. This enables the bosonic microstate $\omega(E, N_{ex}, N)$ to be expressed in terms of the macrostate $\Omega(E, N)$, which is easier to be determined in comparison. As a result, the number fluctuation may be found without the knowledge of the microstate, and thus the computation is speeded up tremendously. The connection to number theory in the bosonic case is possible because the energy spectrum of a one-dimensional harmonic trap is equally spaced, and the N_{ex} bosons are excited from *a single lowest energy level.* On the other hand, the fermionic ground state consists of N energy levels, and this prevents a direct connection to number partitioning theory. It is well known, however, that in one dimension a fermionic problem may be transmuted into a bosonic one, whether the gas is interacting, as in the Luttinger liquid model [61], or noninteracting, as discussed in Ref. [62]. The Fermi-Bose duality has also been shown in (1+1) dimensions [63, 64, 65]. This bosonization property in one dimension strongly suggests that there must be some means, albeit indirect, by which a similar relationship between the microstate and macrostate for fermions in a one-dimensional harmonic spectrum may be established. This shall be, in fact, presented in this section. First, we shall review the bosonic problem in section 4.1.1 to simplify the discussion on fermions, which is to be discussed in section 4.1.2.

4.1.1 Bosons in a one-dimensional harmonic trap

We have seen from previous chapters that the problem of distributing N_{ex} bosons over a set of single-particle excited levels given an energy E is equivalent to partitioning an integer $E = n$ into smaller parts. Because $N_{ex} \leq N$ always, if $N \to \infty$ then there is essentially no restriction on the size of the partitions. The problem then pertains to unrestricted integer partitioning. It is restricted integer partitioning otherwise. The microstate $\omega(E, N_{ex}, N)$, which denotes the number of ways of distributing E quanta over exactly N_{ex} particles, is equivalent to the number of partitions of an integer E into N_{ex} parts. To make the discussion more complete, we shall again go over the example in section 1.1, Fig. 1.1b even though this has already been done at the beginning of chapter 3. In the example, the spectrum is that of a one-dimensional harmonic trap with $N = 3$ and $E = 5$. The first partition of 5, *i.e.*,

$$5 = 5$$

corresponds to the first configuration in which $N_{ex} = 1$ bosons takes up all 5 quanta and excites to the fifth level above the ground state. Thus

$$\omega(5, 1, 3) = 1.$$

The next two configurations with $N_{ex} = 2$ correspond to the partitions

$$5 = 1 + 4,\ 2 + 3,$$

and the last two with $N_{ex} = 3$ correspond to

$$5 = 1 + 1 + 3,\ 1 + 2 + 2.$$

Thus, respectively,

$$\omega(5, 2, 3) = 2,$$

and

$$\omega(5, 3, 3) = 2.$$

The macrostate is

$$\Omega(5, 3) = \sum_{N_{ex}=1}^{3} \omega(5, N_{ex}, 3) = 5.$$

In words, $\Omega(5, 3)$ is the number of partitions of 5 *up to* 3 parts. In order to differentiate from the fermionic microstate to be discussed later, we shall henceforth attach a superscript B for bosons, or F for fermions in $\omega(E, N_{ex}, N)$. After obtaining the bosonic microstate for all excitation energy E, the microcanonical ground state number fluctuation may be found using Eqs. (2.3), (2.4), and (2.7). Obviously this is a cumbersome and therefore not desirable method of determining the microstate. Fortunately, an identity in number theory provides another way of finding the microstate [51]:

$$\begin{aligned} \omega^B(n,k,N) &= \Omega(n-k,k), \ n \geq k, \\ &= 0, \qquad\qquad otherwise. \end{aligned} \tag{4.1}$$

In words, Eq. (4.1) states: *The number of partitions of n into k parts is equal to the number of partitions of $n-k$ into parts not exceeding k.* For instance, consider $k = 2$ from our example above, then the identity reads

$$\omega^B(5,2,3) = \Omega(3,2).$$

Since $3 = 3,\ 1+2$; so $\Omega(3,2) = 2$ which is the same as $\omega^B(5,2,3) = 2$. For $k = 3$, we have

$$\omega^B(5,3,3) = \Omega(2,3),$$

and since $2 = 2,\ 1+1$; $\Omega(2,3) = 2$ which is again the same as $\omega^B(5,3,3) = 2$. Note that Eq. (4.1) implies that $\omega^B(n,N_{ex},N) = \omega^B(n,N_{ex},M), N_{ex} \leq min\{N,M\}$, *i.e.*, changing the system size does not affect the microstates for $N_{ex} \leq min\{N,M\}$. This can be clearly seen from our example. If $N = 4$ instead of 3, then the next admissible partition of 5 is $1+1+1+2$, and the microstates are

$$\begin{aligned} \omega^B(5,1,4) &= 1 = \omega^B(5,1,3), \\ \omega^B(5,2,4) &= 2 = \omega^B(5,2,3), \\ \omega^B(5,3,4) &= 2 = \omega^B(5,3,3), \\ \omega^B(5,4,4) &= 1. \end{aligned}$$

This brings us to an another identity [51]:

$$\omega^B(n,N_{ex},N) = \Omega(n,N_{ex}) - \Omega(n,N_{ex}-1). \tag{4.2}$$

This property was in fact used by the authors in Ref. [9, 26] to calculate an analytic formula for the ground state number fluctuation of bosons as a function of temperature. We shall see shortly, however, that the identity given by Eq. (4.1) is more useful when we discuss the fermionic case in the next section.

4.1.2 Fermions in a one-dimensional harmonic trap

To understand why the fermionic ground state levels prevent direct application of number theory, consider an example similar to the one for bosons given in previous section with $E = 5$ and $N = 3$. Each state is filled with one single fermion which is assumed to be spinless. This assumption corresponds to the spin-polarized fermions in experimental setting where only one spin orientation is confined by the magnetic trap. The microstates are drawn in Fig. 4.1. Note that the ground state consists of three lowest levels. Unlike the bosonic case, there are 3 distinct configurations corresponding to $N_{ex} = 1$, and there is no configuration for $N_{ex} = 3$ since it takes at least $E = 9$ quanta to excite all 3 fermions.

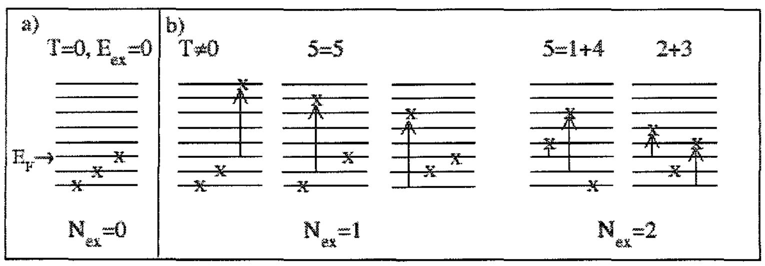


Figure 4.1: Illustration of the fermionic microstates for a harmonic spectrum with $E = 5$, and $N = 3$. a) The particles occupy the lowest states up to Fermi level, denoted by E_F. b) An energy of $E = 5$ quanta are shared amongst the particles which are then excited to the levels above E_F. The partitions of 5 for each configuration are shown on the top. Upward arrows indicating the transitions to higher states are also drawn to guide the eye. Note that the higher energy levels are not shown.

Thus the microstates are:

$$\begin{aligned} \omega^F(5,1,3) &= 3, \\ \omega^F(5,2,3) &= 2, \\ \omega^F(5,3,3) &= 0. \end{aligned}$$

Note that as expected, the macrostate is the same as the bosonic one,

$$\Omega(5,3) = \sum_{N_{ex}=1}^{3} \omega^F(5, N_{ex}, 3) = 5 = \sum_{N_{ex}=1}^{3} \omega^B(5, N_{ex}, 3).$$

If the system size were 4 instead of 3, then clearly there would be 4 ways of exciting one particle,

$$\omega^F(5,1,4) = 4 \neq \omega^F(5,1,3) = 3,$$

in contrast to the bosonic case where the microstate remains the same. This is obviously due to the fact that the fermionic ground state consists of N energy levels instead of a single one, as is the case for bosons. Thus, for fermions relations (4.1) and (4.2) do not apply.

It may be noted that due to Pauli principle the distribution of particles above the fermi level E_F resembles the *distinct* partitions of an integer n. Direct application of the theory is not possible, however, due to complications caused by the fermionic multi-level ground state. This strongly suggests that we treat the fermionic energy levels separately. We proceed as followed. Given n quanta of energy, consider breaking up n into two parts:

$$n = n_h + n_p, \tag{4.3}$$

where n_h is the number of quanta it takes to bring N_{ex} particles to the fermi level E_F (which is equivalent to the distribution of N_{ex} holes to the states below and including E_F), and n_p is the number of quanta it takes to distribute these N_{ex} particles in the excited states above E_F. This effectively divides the fermionic energy levels into two sectors: the *particle space* above E_F and the *hole space* below and including E_F. Let $\omega_h^F(n_h, N_{ex}, N)$ be the number of ways to distribute N_{ex} holes in the hole space, and $\omega_p^F(n_p, N_{ex}, N)$ the number of ways to distribute N_{ex} particles in the particle space, both according to Pauli principle. Then given n quanta and N_{ex} particles,

$$\omega^F(n, N_{ex}, N) = \sum_{\{n_h, n_p\}} \omega_h^F(n_h, N_{ex}, N)\ \omega_p^F(n_p, N_{ex}, N), \tag{4.4}$$

where the set $\{n_h, n_p\}$ satisfies Eq. (4.3) for a given n. The problem now pertains to finding $\omega_h^F(n_h, N_{ex}, N)$ and $\omega_p({}^F n_p, N_{ex}, N)$. At first glance this seems to be more complicated than finding a single quantity $\omega^F(n, N_{ex}, N)$. However, recall that $\omega^F(n, N_{ex}, N)$ is the number of ways of distributing N_{ex} particles above E_F with respect to *a set of* N ground state energy levels. By breaking up the fermionic energy levels into two parts we are now distributing N_{ex} particles above E_F and N_{ex} holes below E_F, *both with respect to a single energy level.* As shall be seen shortly, this allows us to map the fermionic problem to a bosonic one, which may be solved using number partitioning theory. Let us now look at these two spaces separately.

Particle space

First we consider the particle space. This space is unbounded starting from the fermi level E_F. We now imagine a system of 'pseudo fermions' in which N_{ex} particles are in the fermi level. These fermions are to be distributed in the particle space. Thus, n_p quanta are distributed among N_{ex} fermions *with respect to only one energy level* E_F. The problem is now similar to the bosonic one, except the distribution of particles must comply with the Pauli principle. In the language of number theory, $\omega_p^F(n, N_{ex}, N)$ is the number of partitions of n into exactly N_{ex} *distinct* parts, with $N_{ex} \leq N$. We have already encountered this quantity in section 3.4. The desired identity is given by Eq. (3.30):

$$\begin{aligned}\omega_p^F(n_p, N_{ex}, N) &= \Omega(n_p - \frac{N_{ex}(N_{ex}+1)}{2}, N_{ex}), \\ &= \Omega(n_p - \triangle_p, N_{ex}). \end{aligned} \tag{4.5}$$

Remarkably, this is the same form as Eq. (4.1) for bosons with the shift N_{ex} in energy replaced by $\triangle_p = N_{ex}(N_{ex}+1)/2$. This shifted energy is in fact the minimum energy it takes to excite N_{ex} particles from E_F,

$$n_p^{min}(N_{ex}) = \frac{(N_{ex}+1)N_{ex}}{2}. \tag{4.6}$$

Note that the partition function of this space is no longer given by that of N fermions in a one-dimensional harmonic trap, whose expansion coefficients are given by the $\Omega(n, N)$ (see Eq. (2.13)). The multiplicity in Eq. (4.5) should therefore be thought of as the bosonic multiplicity. This notion is most helpful when we discuss the hole space. In other words, the problem is now mapped onto a similar bosonic problem, with the restriction that the parts of an integer being partitioned are *distinct*.

Hole space

We now consider taking N_{ex} particles out of the multi-level ground state and put them in the fermi level E_F (or equivalently, creating N_{ex} holes in the ground state). Given n_h quanta, we wish to find $\omega_h^F(n_h, N_{ex}, N)$, the number of ways of doing this. Unlike the particle space, the dimension of the hole space is bounded, set by the number of particles N of the system. For a given number N_{ex} of particles, the $\mathcal{H}$ilbert space dimension of available states for N_{ex} holes is dependent on the value of N_{ex} itself and is given by:

$$N_{\mathcal{H}} = N - N_{ex}. \tag{4.7}$$

We need to find the partition function of this space for each N_{ex}, and derive a formula similar to Eq. (4.5) for $\omega_h^F(n_h, N_{ex}, N)$. This may be done by considering a new system *containing N_{ex} bosons*, whose energy space is bounded and is given by $N_{\mathcal{H}} + 1$ levels including the ground state, which is set at zero energy. The goal is to determine $Z^h_{N_{ex}}(\beta)$, the *bosonic* partition function for the hole space, and expand this in terms of the coefficient $\Omega_h(n_h, N_{ex})$ as in Eq. (2.13). We have attached a subscript 'h' in $\Omega_h(i, N_{ex})$ to differentiate from that of the particle space. Using the recursion formula Eq. (2.17), the N_{ex}-hole partition function of this hypothetical system is

$$Z^h_{N_{ex}}(\beta) = \frac{1}{N_{ex}} \sum_{j=1}^{N_{ex}} Z_1^h(j\beta) Z^h_{N_{ex}-j}(\beta), \tag{4.8}$$

where $Z_1^h(\beta)$ is the one-particle partition function of the system containing N_{ex} bosons and is given by:

$$Z_1^h(\beta) = \sum_{i=0}^{N_{\mathcal{H}}} e^{-\beta i}. \tag{4.9}$$

It is important to stress that the one-particle partition function needs to be determined for each N_{ex}, and $Z^h_{N_{ex}}(x)$ may then be found from (4.8). The $Z^h_{N_{ex}}(x)$ is now the generating functions of $\Omega_h(n, N_{ex})$:

$$Z^h_{N_{ex}}(x) = \sum_i \Omega_h(i, N_{ex}) x^i, \tag{4.10}$$

where, as before, x is a mathematical parameter < 1. We are now ready to determine a formula for $\omega_h^F(n_h, N_{ex}, N)$. Because the hole space includes E_F, the minimum energy to create a hole (or dig a particle) and put it in the fermi level is zero, since there already is a particle there; for two holes the minimum energy is one, for three holes it is three, etc. In general,

$$n_h^{min}(N_{ex}) = \frac{(N_{ex}-1)N_{ex}}{2}. \tag{4.11}$$

Similar to Eq. (4.5), with the energy shift Δ_h given by (4.11), the number of ways of creating N_{ex} holes in the hole space $\omega_h^F(n_h, N_{ex}, N)$ is given by:

$$\omega_h^F(n_h, N_{ex}, N) = \Omega_h(n_h - \frac{N_{ex}(N_{ex}-1)}{2}, N_{ex}). \tag{4.12}$$

Using Eqs. (4.5) and (4.12), the number of ways of distributing N_{ex} fermions to the excited states, Eq. (4.4), now reads

$$\omega^F(n, N_{ex}, N) = \sum_{\{n_h, n_p\}} \Omega(n_p - \frac{N_{ex}(N_{ex}+1)}{2}, N_{ex})\ \Omega_h(n_h - \frac{N_{ex}(N_{ex}-1)}{2}, N_{ex}). \tag{4.13}$$

It is obvious that if there is no hole space, $\omega_h^F(n_h, N_{ex}, N) = \Omega_h(n_h - \Delta_h, N_{ex}) = 1$, the sum over the set $\{n_h, n_p\}$ vanishes since $n = n_p$, the energy shift $\Delta_p = n_p^{min}(N_{ex}) = N_{ex}$, and Eq. (4.4) thus reduces to Eq. (4.1) for bosons.

As an illustration, let us use Eq. (4.13) to calculate $\omega^F(5,1,3)$, $\omega^F(5,2,3)$, and $\omega^F(5,3,3)$, already determined at the beginning of this section by direct counting. The bosonic partition function in power of x for the particle space for $N_{ex} = 1, 2, 3$ are:

$$\begin{aligned}
Z_1 &= 1 + x + x^2 + x^3 + x^4 + x^5 + \ldots, \\
Z_2 &= 1 + x + 2x^2 + 2x^3 + 3x^4 + 3x^5 + \ldots, \\
Z_3 &= 1 + x + 2x^2 + 3x^3 + 4x^4 + 5x^5 + \ldots,
\end{aligned}$$

where the coefficients of x are the macrostates $\Omega(n, N)$. These partition functions may be obtained from expanding the function

$$Z_{N_{ex}} = \prod_{m=1}^{N_{ex}} \frac{1}{1 - x^m}$$

in power of x. Next, the bosonic partition functions for the hole space are:

$$\begin{aligned}
Z_1^h &= 1 + x + x^2, \\
Z_2^h &= 1 + x + x^2, \\
Z_3^h &= 1.
\end{aligned}$$

Note that these partition functions are finite since the Hilbert space dimension of the hole space is finite. Also, due to symmetry, $Z_i^h = Z_{N-i}^h$. Using Eq. (4.13), therefore,

$$\begin{aligned}
\omega^F(5,1,3) &= \Omega(0,1)\Omega_h(4,1) + \Omega(1,1)\Omega_h(3,1) + \Omega(2,1)\Omega_h(2,1) + \\
&\quad \Omega(3,1)\Omega_h(1,1) + \Omega(4,1)\Omega_h(0,1), \\
&= (1)(0) + (1)(0) + (1)(1) + (1)(1) + (1)(1), \\
&= 3,
\end{aligned}$$

which is what we obtained before by directly enumerating the microstates. Similarly,

$$\begin{aligned}
\omega^F(5,2,3) &= \Omega(-2,2)\Omega_h(3,2)+\Omega(-1,2)\Omega_h(2,2)+\Omega(0,2)\Omega_h(1,2)+\Omega(1,2)\Omega_h(0,2),\\
&= (0)(0)+(0)(1)+(1)(1)+(1)(1),\\
&= 2,\\
\omega^F(5,3,3) &= \Omega(-5,3)\Omega_h(1,3)+\Omega(-4,3)\Omega_h(0,3)+\Omega(-3,3)\Omega_h(-1,3)+\\
&\quad \Omega(-2,3)\Omega_h(-2,3),\\
&= 0. \qquad (4.14)
\end{aligned}$$

Since the multiplicities are zero for $n < 0$, it is more computational convenient to define $n_{cutoff} \equiv n_h^{max} - n_h^{min} = n - N_{ex}{}^2$, then Eq. (4.13) becomes

$$\omega^F(n, N_{ex}, N) = \sum_{i=0}^{n_{cutoff}} \Omega(i, N_{ex})\Omega_h(n_{cutoff} - i, N_{ex}). \qquad (4.15)$$

In appendix C we give a list of the (bosonic) partition functions for both the particle and hole spaces for $N = 10$. Also shown are computer algorithms for computing the microstates using the method described in this section. The mathematical program used is Maple V.

In Ref. [25] where the direct combinatorial method was used, the fermionic calculation of the ground state fluctuation was restricted to a low number of particles N and quanta n using a normal office computer (Pentium III, 500 MHz). For a relatively small number of particles (*e.g.*, $N = 10$), at higher excitation n the combinatorics method is more time-consuming due to the rapid increase in the number of possibilities with n. The method described in this section translates the problem in combinatorics into a problem of calculating the partition functions of the hole space, the latter being simpler computationally. Although this method is still time-consuming and the calculation for larger N ($N \geq 100$) is still not possible using our office computer, it is more effective for higher number of quanta and relatively small number of particles. For demonstration we display the ground state fluctuation of fermions as a function of energy quanta n in Fig. 4.2 for $N = 30$. We also show the corresponding curve in CE, which is the same as GCE except at very low temperature (see *e.g.*, Ref. [25]) for comparison. As expected, both go to zero as $T \to 0$, with the microcanonical fluctuation less than that given by the CE for all n. Note that the two fluctuations are very different, even for very high excitations. At $n = 6000$ which is

$200 \times E_F$, the canonical curve still differs from the microcanonical one by about 14%. It was shown in Ref. [25] for $N = 15$ that the ground state occupancy $\langle N_0 \rangle = \sum_k^{E_F} \langle n_k \rangle$ for the two ensembles are very similar. Clearly, the number fluctuation is more sensitive to the ensemble used. Therefore, for a relatively small particle number, while it may be adequate to use the CE (or GCE) to describe a thermodynamic quantity such as the ground state occupancy, it should be used with caution when calculating the number fluctuation and related quantities.

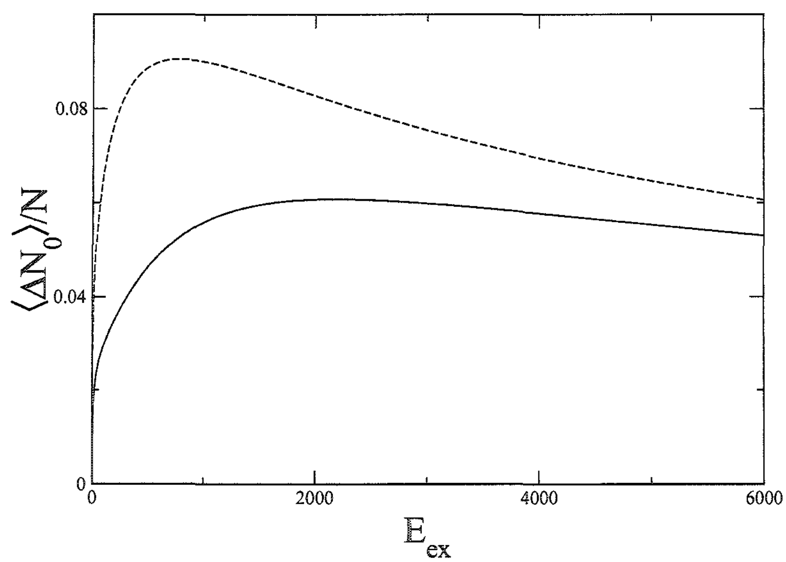


Figure 4.2: Ground state number fluctuation of fermions as a function of excitation energy E (in unit of $\hbar\omega$) for $N = 30$ (solid line). The result in the CE (dashed line), calculated using the method outlined in section 2.1.2, is also shown for comparison.

4.2 The Special Traps

We have seen that for bosons the use of the CE or the more restricted MCE produces the correct ground state number fluctuation as $T \to 0$, while the GCE gives unphysical result. With respect to the number fluctuations, therefore, the GCE is neither thermodynamically equivalent to the CE nor to the MCE, where the total number of particles N is fixed and is not subject to fluctuations. The fluctuations in the latter two ensembles have been shown to respect the principle of thermodynamic equivalence in a one-dimensional harmonic trap but they differ in higher dimensions [9, 11, 15, 16, 17]. A good discussion on the difference between the CE and MCE is given in Ref. [17]. While the number fluctuation is sensitive to the ensemble used, the mean number in the ground state, however, is found to be thermodynamically the same in all statistical ensembles.

In this section we consider a system of noninteracting particles in hypothetical traps whose energy spectra are given by $\ln p$, where p is a prime number, and $\ln n$, where n is an integer. Because of the peculiarity of the spectra, the usual thermodynamic equivalence is not obeyed here. These spectra serve as exceptions to the general rule and therefore are of some interest. In the previous section we encountered an example of the *additive* number theory being applied to a physics problem, in this section it is the *multiplicative* number theory that plays a role.

4.2.1 $\ln p$ spectrum

Fluctuation in the microcanonical ensemble

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

$$\epsilon_p = \ln p, \tag{4.16}$$

where p runs over the prime numbers $2, 3, 5, \ldots$. Suppose that there are N bosons in the ground state at zero energy, and an excitation energy E_{ex} is given to the system. We would like to know in how many ways this energy can be shared amongst the bosons by this spectrum. Recall that as long as $N > E_{ex}$, the enumeration is insensitive to the value of N. In what follows we shall not specify N, and assume that it is large. For $E_{ex} = \ln 2$, only one particle gets excited to the first level above the ground state. Thus,

$\omega(\ln 2, 1, N) = 1$, $\omega(\ln 2, N_{ex}, N) = 0$, for $N_{ex} > 1$, and $\Omega(\ln 2, N) = 1$. Similarly for $E_{ex} = \ln 3$. For $E_{ex} = \ln 4$, there cannot be one excited particle, since the energy level with $\epsilon = \ln 4$ does not exist. The only case possible is to excite two particles. Since $\ln 4 = 2 \ln 2$, these two particles both get excited to the level with energy $\epsilon = \ln 2$. Thus $\omega(\ln 4, 1, N) = 0$, $\omega(\ln 4, 2, N) = 1$, $\omega(\ln 4, N_{ex}, N) = 0$, for $N_{ex} > 2$, and $\Omega(\ln 4, N) = 1$. Clearly, for a given excitation energy $E_{ex} = \ln n$, where n is integer, the multiplicity $\Omega(E_{ex}, N)$ equals the number of ways $\ln n$ may be expressed as sums of $\ln p$, where p is prime. This is the same as the number of ways that an integer n may be expressed as a product of prime numbers. Without doing any calculation, we know the answer. According to the *fundamental theorem of arithmetic* [1], there is only one unique way of expressing n as a product of primes:

$$n = p_1^{n_1} p_2^{n_2} \dots p_r^{n_r} \dots, \tag{4.17}$$

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. (4.17) that if the excitation energy $E_{ex} = \ln\ n$, where the integer $n \geq 2$, there is only one unique way of exciting the particles from the ground state. Note that if $E_{ex} \neq \ln n$, the energy is not absorbed by the quantum system. Since the number of bosons excited from the ground state is unique for this system, the microcanonical number fluctuation in the ground state is *identically zero* for any excitation energy. In table 4.1 we list the microstate and the macrostate for a few excitation energies. As expected, the macrostate is always equal to unity.

Fig. 4.3 shows a graph of the excited particles $\langle N_{ex} \rangle$, calculated using Eq. (2.3), versus excitation energy E_{ex}. For clarity we present $\langle N_{ex} \rangle$ instead of $\langle N_0 \rangle$ since N_{ex} is equal to the number of prime factors of integer n. The number of ground state particles may be easily calculated using $\langle N_0 \rangle = N - \langle N_{ex} \rangle$. Due to the peculiarity of the $\ln\ p$ quantum spectrum, the graph has an interesting zigzagging pattern. Note that the result here is independent of N. We shall see in the next section that this result is dramatically different from the smooth one obtained from the CE.

[1]Proven by Euclid ($\sim$ 325-265 BC) around 300 BC.

E_{ex}		N_{ex}	$\omega(E_{ex}, N_{ex}, N)$	$\Omega(E_{ex}, N)$
$\ln 2$		1	1	1
$\ln 3$		1	1	1
$\ln 4$		1	0	
	$= 2\ln 2$	2	1	1
$\ln 5$		1	1	1
$\ln 6$		1	0	
	$= \ln 2 + \ln 3$	2	1	1
$\ln 7$		1	1	1
$\ln 8$		1	0	
		2	0	
	$= 3\ln 2$	3	1	1
$\ln 9$		1	0	
	$= 2\ln 3$	2	1	1
$\ln 10$		1	0	
	$= \ln 2 + \ln 5$	2	1	1
	$\vdots$	$\vdots$	$\vdots$	1

Table 4.1: Enumeration of the microstate $\omega(E_{ex}, N_{ex}, N)$ and the macrostate $\Omega(E_{ex}, N)$ for a few excitation energies for N bosons. The single-particle spectrum is taken as $\epsilon_p = \ln\ p$, where p is prime number sequence. The ground state is at zero energy. Note that in the last row, the value of the macrostate in the last column is always equal to 1 regardless of the values of the first 3 columns.

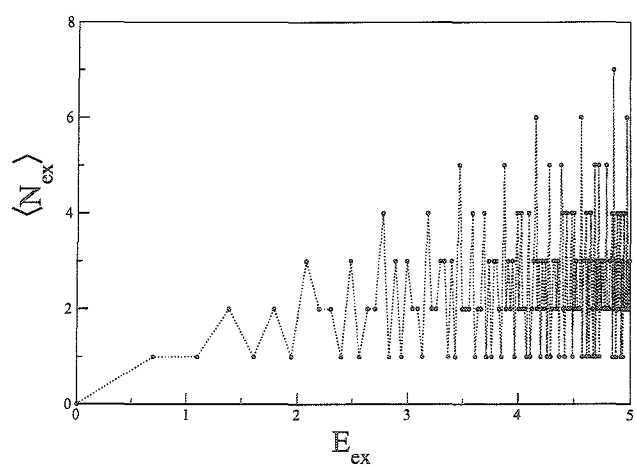
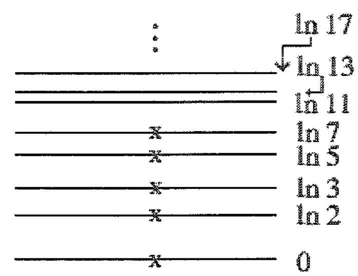


Figure 4.3: Plot of the average bosonic occupancy in the excited states $\langle N_{ex} \rangle$ as function of $E_{ex} = \ln\ n$, where n is an integer. The data points are joined by dotted lines to emphasize their zigzag character. To give an example, the sixth point (including 0) corresponds to $E_{ex} = \ln 6$, and gives $N_{ex} = 2$, corresponding to the prime factor decomposition 2×3.

We next ask what happens to the microcanonical ground state number fluctuation in the presence N ideal fermions. While the distribution of the excitation energy is more constrained due to Pauli principle, the N-level fermionic ground state might allow more possibilities, which might render the fluctuation to be non-zero. To examine what the case might be, we consider an example with $N = 5$. The ground state of this system consists of five lowest energy levels as shown:



To excite one particle, one needs an excitation energy of

$$E_{ex} = \ln\ p - \ln\ p^0 = \ln\ \frac{p}{p^0},$$

where

$$p > 7,\ p^0 = \varepsilon\{1, 2, 3, 5, 7\}.$$

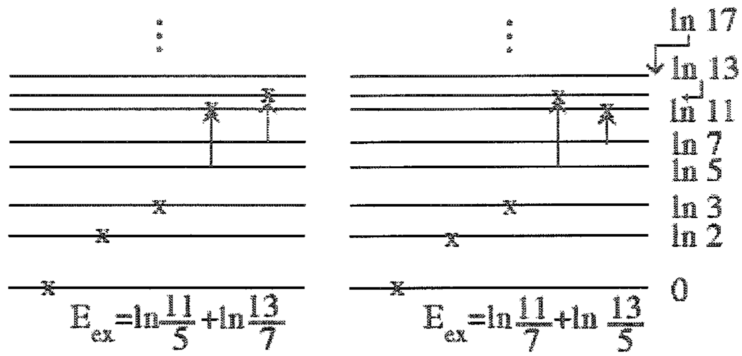
For instance, for $E_{ex} = \ln \frac{11}{7}$, the particle in the Fermi level ($E_F = \ln 7$) will be excited to the first excited level with $\epsilon = \ln 11$. For each excitation energy given by $\ln\ p/p^0$, there is only one way of exciting one particle. For two particles, the energy required is

$$E_{ex} = \ln \frac{p_1}{p_1^0} + \ln \frac{p_2}{p_2^0},$$

where

$$p_1 \neq p_2\ \&\ \{p_1, p_2\} > 7,\ p_1^0 \neq p_2^0\ \&\ \{p_1^0, p_2^0\} = \varepsilon\{1, 2, 3, 5, 7\}.$$

An example is $E_{ex} = \ln\frac{11}{7} + \ln\frac{13}{5}$. Note that this is equivalent to $\ln\left(\frac{11}{7}\frac{13}{5}\right) = \ln\left(\frac{13}{7}\frac{11}{5}\right) = \ln\frac{13}{7} + \ln\frac{11}{5}$, both *belongs to the same configuration* as shown:



Even though each particle absorbs different energies in two pictures, the final configurations are identical since the particles are indistinguishable. Therefore, $\Omega(\ln\left(\frac{11}{7}\frac{13}{5}\right), N) = 1$.

In general, for N fermions, the excitation energy is of the form

$$\begin{aligned} E_{ex} &= \ln\frac{p_1}{p_1^0} + \ln\frac{p_2}{p_2^0} + \ldots, \\ &= \ln\left[\frac{\prod_{i=1}^{N_{ex}} p_i}{\prod_{i=1}^{N_{ex}} p_i^0}\right], \end{aligned} \tag{4.18}$$

where the p_i and p_i^0 must be *distinct* due to Pauli principle. Since they are distinct primes, the ratio inside the square bracket of Eq. (4.18) is irreducible and is thus unique. In other words, if $n_1 = \prod_{i=1}^{N_{ex}} p_i$ and $n_2 = \prod_{i=1}^{N_{ex}} p_i^0$, then there is no other n_1' and n_2' such that

$$\frac{n_1'}{n_2'} = \frac{n_1}{n_2}$$

unless $n_1 = n_1'$ and $n_2 = n_2'$. Compared to the bosonic case, there are more energies that are not absorbed by the quantum spectrum. The inadmissible energies are those that cannot be expressed as $\ln\ n$, and those that do not satisfy Eq. (4.18). Since there is one unique way, if possible, of expressing E_{ex} as $\ln(n_1/n_2)$, the fermionic microcanonical ground state number fluctuation is also identically zero at all excitation energies.

Fluctuation in the canonical and grand-canonical ensembles

We next calculate the fluctuation in the CE and GCE for N bosons and compare with the microcanonical results. To do the numerical work, we need to truncate the spectrum. The canonical one-body partition function is then given by

$$Z_1(\beta) = 1 + \sum_{p=2}^{p^*} \exp(-\beta \ln p), \tag{4.19}$$

where p^* is the cutoff prime. The N-body partition function may be found using Eq. (2.17). Once $Z_N(\beta)$ is found, the canonical ground state occupation and the ground state number fluctuation can be readily computed from Eqs. (2.18)-(2.20).

In the MCE the ground state occupancy and the fluctuation are calculated exactly, and the energy is well defined. In the CE, however, the system is in thermal equilibrium with a heat reservoir, the energy is therefore defined only in the average sense. For a given temperature T, the most probable energy of the system in the CE is

$$\langle E_{ex} \rangle = -\frac{\partial \ln Z_N(\beta)}{\partial \beta}. \tag{4.20}$$

The calculations in the CE are thus done for a *range* of energy of finite width, the peak of which is given by (4.20). Therefore, the CE effectively samples more than one energy level at a time. The multiplicity is thus no longer unity and the fluctuation is non-zero. In Figs. 4.4 and 4.5, we display the results of the canonical calculations (solid lines) for the ground state occupancy fraction $\langle N_0 \rangle / N$ and the ground state fluctuation $\langle \triangle N_0 \rangle / N$ for $N = 100$ as a function of temperature T with the truncated spectrum of 10^6 primes. For comparison, we also show the results of the corresponding grand canonical calculations (dashed lines). The grand canonical quantities are calculated from Eqs. (2.22) and (2.24). Interestingly, the ground state occupation graph appears to have a transition temperature, and shows signature of BEC. We defer the discussion on this later so that the subject on fluctuation is not interrupted. While the average ground state occupancy in the two ensembles agree quite well, the grand canonical catastrophe for the number fluctuation is clearly evident.

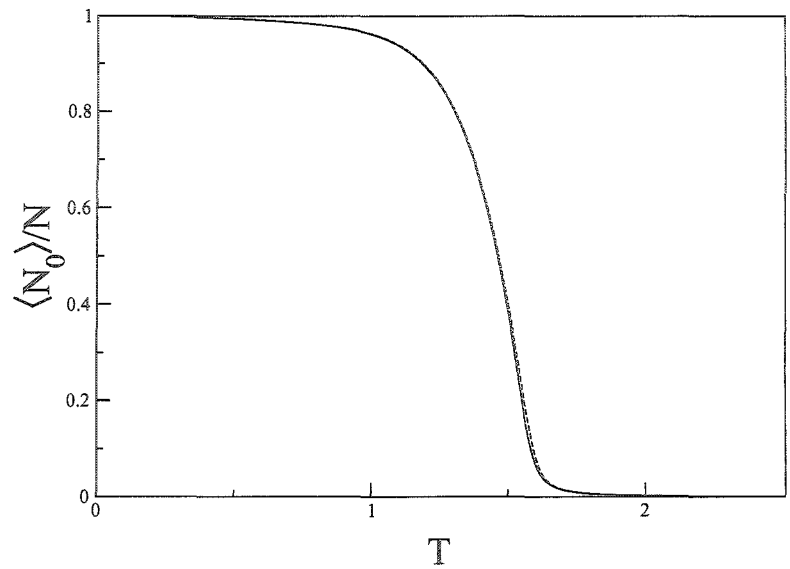


Figure 4.4: Average occupancy in the ground state $\langle N_0 \rangle / N$ versus temperature T for $N = 100$ in the canonical (solid line) and grand canonical (dashed line) ensembles. The spectrum is truncated to 10^6 primes.

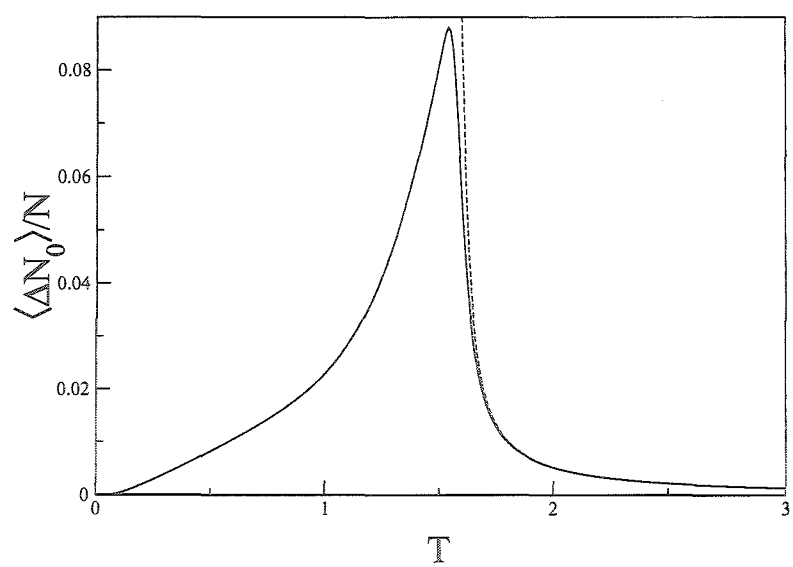


Figure 4.5: Plot of the relative ground state number fluctuation in the canonical (solid line) and the grand canonical (dashed line) ensembles for the truncated spectrum of 10^6 primes. Note the steep rise in the grand canonical fluctuation.

Clearly, the canonical fluctuation does not vanish except at zero temperature. This result is dramatically different from the microcanonical one which is zero everywhere.

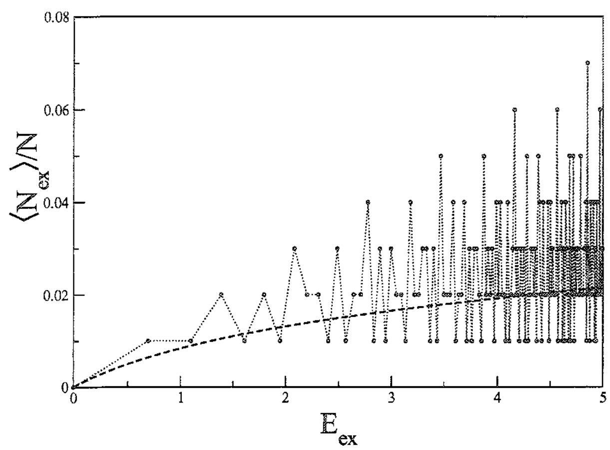


Figure 4.6: Same as Fig. 4.3 except with the canonical curve (dashed line) superimposing for comparison. For the canonical calculation, the ensemble-averaged $\langle E_{ex} \rangle$ is identified with the excitation energy E_{ex}. Note that the microcanonical result is identical to the previous shown in Fig. 4.3 ($N \to \infty$). This is because at this scale of the excitation energy, the number of factors of n is still $\ll N = 100$.

We next compare the fraction of number of particles in the excited states $\langle N_{ex} \rangle / N$ in the MCE and CE for the same number of particles. This is displayed in Fig. 4.6, which shows that the two results are dramatically different. While the canonical ratio $\langle N_{ex} \rangle / N$ keeps on increasing for larger E until it saturates at unity, the zigzagging pattern of the microcanonical result will still persists no matter how large the energy is. In particular, whenever $E_{ex} = \ln p$, the microcanonical ratio $\langle N_{ex} \rangle / N$ will always be equal to 0.01. This means that the microcanonical result can never be smooth.

We expect the same conclusion holds true for fermions. The fermionic ground state number fluctuation in the CE will be smooth and non-zero except at zero temperature. The microcanonical ratio $\langle N_{ex} \rangle / N$ will still show the zigzagging pattern, though the magnitude will be less than the bosonic case due to Pauli principle.

The next question to be addressed is whether the same outcome holds if the spectrum is not cut off and the number of particles $N \to \infty$. Since $N \to \infty$, the number of factors is not restricted. The many-body energy is given by $\ln n$, and the degeneracy is always unity. The canonical partition function is thus given by

$$Z_N(\beta) = \sum_E e^{-\beta E} = \sum_{n=1}^{\infty} e^{-\beta \ln n} = \sum_{n=1}^{\infty} \frac{1}{n^\beta}. \tag{4.21}$$

This is nothing but the well known Riemann zeta function,

$$Z_N(\beta) = \zeta(\beta) = \sum_n \frac{1}{n^\beta}, \tag{4.22}$$

It is to be noted that mathematically the zeta function may be analytically continued on the complex β plane. Nontrivial zeros on the complex plane are believed to lie only on the real $\beta = 1/2$ axis. This is known as the Riemann hypothesis, which is yet to be proven. For real β Eq. (4.22) converges for $\beta > 1$. Thus this system may only be realized at low temperatures. We have encountered the generating functions in additive number theory (see table 2.1 and chapter 3). Likewise, the zeta function is a multiplicative generating function, with all the degeneracy factors being unity. This system of a collection of bosonic gas in $\ln p$ spectrum, referred to as *Riemann* gas, was first introduced by Julia [33] who thereby made a connection between a quantum mechanical system and a mathematical entity, namely the zeta function. Henceforth we shall concern only with the region $\beta > 1$. Note that the problem of divergence in the partition function did not arise earlier because the spectrum was cut off. The grand canonical partition function of this system may also be determined:

$$\begin{aligned}
\Xi(\beta,\mu) &= \prod_{\epsilon_i} \frac{1}{1-e^{\beta(\mu-\epsilon_i)}}, \\
&= \frac{1}{1-e^{\beta\mu}} \prod_{p=2}^{\infty} \frac{1}{1-e^{\beta(\mu-\ln p)}}, \\
&= \frac{1}{1-e^{\beta\mu}} \prod_{p=2}^{\infty} \frac{1}{1-e^{\beta\mu}\frac{1}{p^\beta}}, \\
&= \frac{1}{1-e^{\beta\mu}}\, \Xi_{ex}(\beta,\mu),
\end{aligned} \tag{4.23}$$

where the factor $\frac{1}{1-e^{\beta\mu}}$ is due to the ground state which is at $\epsilon_0 = \ln 1 = 0$ energy, and $\Xi_{ex}(\beta,\mu) \equiv \prod_{p=2}^{\infty} \frac{1}{1-e^{\beta\mu}/p^\beta}$ is the grand partition function of the excited states. Note that $\Xi_{ex}(\beta,\mu)$ with $\mu = 0$ is none other than the Euler product representation of the Riemann zeta function [66]:

$$\zeta(\beta) = \sum_n \frac{1}{n^\beta} = \prod_p^{\infty} \frac{1}{1-\frac{1}{p^\beta}}. \tag{4.24}$$

The corresponding gas for non-zero μ is termed Riemann-Beurling gas [34]. To address the question raised earlier, *i.e.*, whether the outcome from the previous case of finite N and a cut-off spectrum still holds for this system where $N \to \infty$ and the spectrum is not cut off, we shall use the method developed by Navez *et al.* [16, 17]. These authors pointed out 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's demon (MD) ensemble. Note that we are not addressing the issue of whether the Riemann gas truly condenses, this shall be discussed later. The treatment here applies as long as $\langle N_0 \rangle$ becomes macroscopic at a temperature, as shown in Fig. 4.4. In this MD ensemble, 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. Defining $\alpha = \beta\mu$, it was shown that the canonical occupancy of the excited states, $\langle N_{ex} \rangle$, and the number fluctuation $\langle \triangle {N_{ex}}^2 \rangle$ could be obtained from the first and the second derivative of $\Xi_{ex}(\beta, \alpha)$ with respect to α, 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

$$\langle \triangle {N_{ex}}^2 \rangle_{MCE} = \langle \triangle {N_{ex}}^2 \rangle_{CE} - \frac{[\langle \triangle N_{ex} \triangle E \rangle_{CE}]^2}{\langle \triangle E^2 \rangle_{CE}}. \tag{4.25}$$

This worked beautifully for harmonic traps in various dimensions. These calculations, for our system, are also easily done for $\beta > 1$:

$$\langle \triangle {N_{ex}}^2 \rangle_{MCE} = \sum_p \frac{p^\beta}{(p^\beta - 1)^2} - \frac{\left[\sum_p \frac{(\ln p) p^\beta}{(p^\beta - 1)^2}\right]^2}{\sum_p \frac{(\ln p)^2 p^\beta}{(p^\beta - 1)^2}} . \tag{4.26}$$

Clearly, the RHS of Eq. (4.26) is non-zero, and therefore *does not agree with the actual microcanonical result.* Remarkably, the canonical partition function Eq. (4.21) is not needed at all for this calculation.

Normally the occupancy is not as sensitive as the number fluctuation with respect to the ensemble used (see *e.g.*, Fig. 4.4). The microcanonical occupancy is generally less than that of the other two ensembles but possesses similar features. To simplify the discussion, we shall focus only on the microcanonical and canonical results. Here, even the occupancies in these two ensembles are dramatically different, not to mention the number fluctuation. This failure of the CE in predicting the MCE results is not a shortcoming of the methodologies, but is due to the exotic nature of the single-particle quantum spectrum. Recall that in the MCE there is one and only one microstate for any given excitation energy. This implies a one-to-one correspondence between the microstate and the macrostate. Since there are not a large number of microstates corresponding to a macrostate, the usual concept of statistical mechanics breaks down. Albeit nonphysical, this quantum spectrum is still a highly interesting example illustrating the non-equivalence of the ensembles.

We now return to the issue of whether bose gas in $\ln p$ spectrum displays BEC. As noted earlier, Fig. 4.4 appears to show a transition temperature T_c below which the ground state occupation becomes macroscopic. The transition is indeed sharper than the one-dimensional harmonic case for the same number of particles, as shown in Fig. 4.7. The transition temperature may be readily found in the GCE using the density of state approach:

$$N - N_0 = \int_0^\infty n(\epsilon)\rho(\epsilon)d\epsilon, \quad (4.27)$$

and letting $N_0 \rightarrow 0$, and the fugacity $z = e^{\mu\beta} \rightarrow 1$ (the energy of the ground state has been taken to be zero). In (4.27), $n(\epsilon) = \left[z^{-1}exp(\epsilon\beta) - 1\right]^{-1}$ is the usual Bose-Einstein occupation number, and $\rho(\epsilon)$ is the single-particle density of states. In the one-dimensional harmonic case, it is well known [67, 68] that BEC does not occur in the thermodynamic limit ($N \rightarrow \infty$ and $\omega \rightarrow 0$ such that $N\omega$ =constant). However, for finite N the system does undergo a 'quasi' BEC (see Fig. 4.7) [9, 69]. In fact, the transition temperature of this system was estimated to be [69]

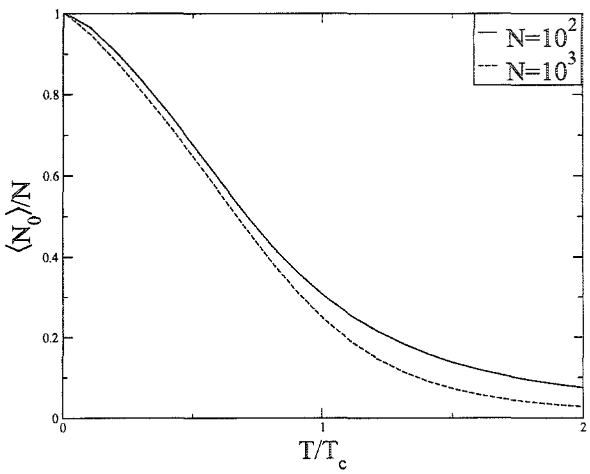


Figure 4.7: The relative ground state occupation for finite number N of bosons in a one-dimensional harmonic potential versus (relative) temperature. Plots are shown for $N = 10^2$ (solid line) and $N = 10^3$ (dashed line).

$$T_c = \hbar\omega\frac{N}{\ln(2N)}. \quad (4.28)$$

Eq. (4.28) was derived using a 'summation' approach which does not require the knowledge of the density of state. The detail of the calculation is shown in appendix D. Since the density of states for the $\ln p$ spectrum is not known, we follow this 'summation' approach.

The total number of particles, Eq. (D.2), is

$$\begin{aligned} N &= \sum_{j=1}^{\infty} z^j \sum_i e^{-j\epsilon_i\beta}, \\ &= N_0 + \sum_{j=1}^{\infty} z^j \sum_{p=2}^{p^*} e^{-j\beta \ln p}, \end{aligned} \tag{4.29}$$

where as before, p^* is the cut-off prime. In the harmonic case, the second summation over the energy level is a geometric progression series (Eq. (D.3)). Here, it cannot be summed, and as a result T_c may not be found analytically. Fig. 4.8 displays $\langle N_0 \rangle /N$ as a function of temperature for several values of N. Clearly, larger number of particles yields larger T_c. However, for a given N, larger value of p^* reduces it. The same behavior can be seen in Fig. 4.9 which shows a plot of the chemical potential μ versus the temperature T. Since the transition is sharper for larger number of particles, we expect the Riemann gas ($p^* \to \infty$ and $N \to \infty$) to exhibit BEC. Recall that this system is realized only for $\beta > 1$, the transition temperature is thus found in the region $T < 1$.

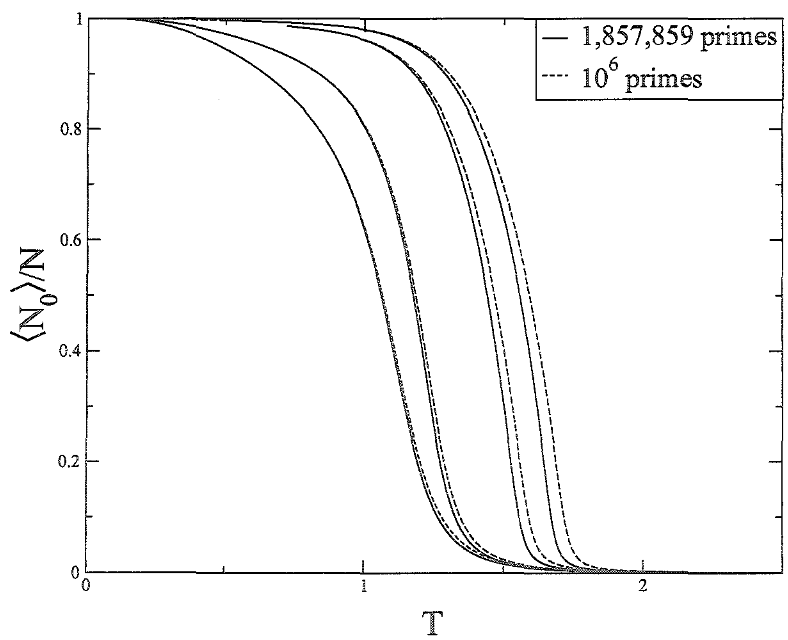


Figure 4.8: Plot of the relative ground state occupation for several N. In order of increasing T, the values of N are $N = 10, 20, 100, 200$. The calculations are done for $p^* = 1,857,859$ and 10^6.

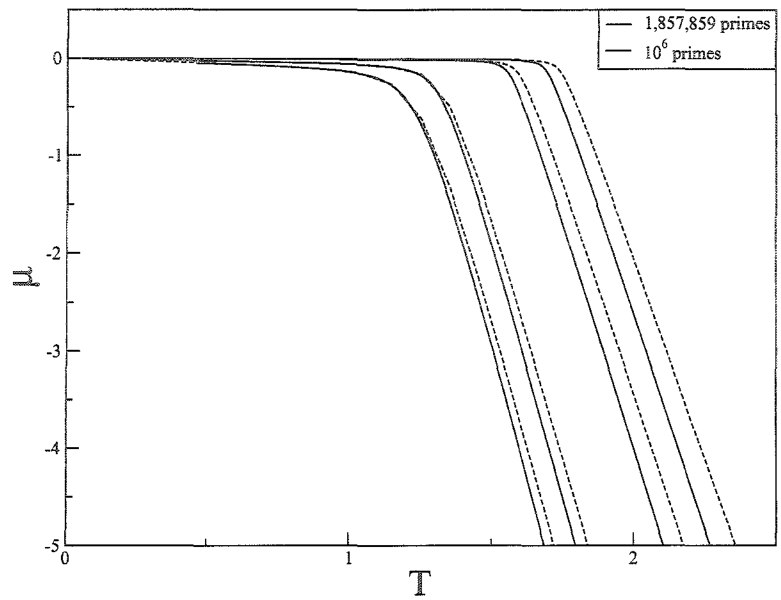


Figure 4.9: Plot of the chemical potential μ versus the temperature T. The number of particles used are the same as in Fig. 4.8.

4.2.2 $\ln n$ spectrum

We next consider a related model in which the single-particle spectrum is given by the logarithm of an integer

$$\epsilon_n = \ln n, \;\; n = 1, 2, \ldots . \tag{4.30}$$

Thus the single-particle partition function is the Riemann zeta function $\zeta(\beta)$. Unlike the $\ln p$ model considered in previous section where a Hamiltonian is not known, it is possible to construct the corresponding dynamical Hamiltonian in this case. This may be done by inferring from the Hamiltonian of a one-dimensional oscillator, which is given by $H = \hat{P}^2 + \hat{Q}^2$, where $\hat{P}$ and $\hat{Q}$ are the momentum and potential operators (in suitably scaled units). The eigenenergy spectrum is $\epsilon_n = (n + 1/2)$, $n = 0, 1, 2, \ldots$ in unit of $\hbar\omega$. Since the eigenvalues of the $\ln n$ model is a function of those of the one-dimensional harmonic oscillator, it follows that the Hamiltonian of the former is given by [70]

$$H = \ln\left(\hat{P}^2 + \hat{Q}^2 + 1\right). \tag{4.31}$$

However, this Hamiltonian is not separable into the usual kinetic and potential operators ($H = \hat{T} + \hat{V}$). Nevertheless, it has been shown in Ref. [70] that the classical partition function derived from this dynamical Hamiltonian yields a good approximation to the canonical partition function $\zeta(\beta)$. Using the WKB semiclassical approximation, it was shown that the potential given by $V \sim \ln r$ in three dimensions yields energy spectrum $E_{nl} \sim \ln(n + l/2 - 1/4)$ [71]. For larger n, these WKB eigenvalues agree better with the exact values found numerically. In one dimension, the potential varies as $V \sim \ln x$ semiclassically produces the eigenenergies $E_n \sim \ln n$.

We now return to the problem of number fluctuation of this spectrum, and compare the results in different ensembles as well as with those of the $\ln p$ single-particle spectrum. We consider N bosons in the ground state at zero energy, where N is large, and calculate the number of ways the excitation energy given by $E_{ex} = \ln n$ is shared amongst the particles. Clearly, in the MCE this problem pertains to finding the number of ways an integer n may be decomposed into N_{ex} factors, where $N_{ex} = 1, 2, \ldots$. In contrast to the $\ln p$ case, there is more than one way of doing this, since the single-particle spectrum given by (4.30) now admits non-prime factorization of n. For illustration we show an example in table 4.2 for a few excitation energies. Since $\Omega(E, N)$ is not always unity, the number fluctuation

E_{ex}	N_{ex}	$\omega(E_{ex}, N_{ex}, N)$	$\Omega(E_{ex}, N)$
$\ln 2$	1	1	1
$\ln 3$	1	1	1
$\ln 4$	1	1	
$= 2\ln 2$	2	1	2
$\ln 5$	1	1	1
$\ln 6$	1	1	
$= \ln 2 + \ln 3$	2	1	2
$\ln 7$	1	1	1
$\ln 8$	1	1	
$= \ln 2 + \ln 4$	2	1	
$= 3\ln 2$	3	1	3
$\ln 9$	1	1	
$= 2\ln 3$	2	1	2
$\ln 10$	1	1	
$= \ln 2 + \ln 5$	2	1	2

Table 4.2: Enumeration of the microstate $\omega(E_{ex}, N_{ex}, N)$ and the macrostate $\Omega(E_{ex}, N)$ for a few excitation energies for N bosons. The single-particle spectrum is taken as $\epsilon_p = \ln\ n$, where n is integer > 1. The ground state is at zero energy.

from the ground state in this case is not always zero. In spite of this, there remains the question of whether the relative ground state number fluctuation in the MCE and the CE asymptotically agree. We shall see shortly that the same conclusion for the $\ln p$ spectrum also holds here. The results of the two ensembles differ no matter how large E and N are. Fig. 4.10 displays a graph of the averaged excited particles $\langle N_{ex}\rangle$ in the MCE, calculated using Eq. (2.3), versus the excitation energy E_{ex}. The calculation is done for only a few excitation energies, since it is not trivial to find the number of factorizations for large values of n. This is actually sufficient for our analysis. The graph in Fig. 4.10 is similar to the one in Fig. 4.3. Due to the fact that the microstates are all non-zero for small values of N_{ex}, the magnitude of $\langle N_{ex}\rangle$ in this case is however smaller (also compare the second and third columns of tables 4.1 with 4.2). Note also that apart from zero $\langle N_{ex}\rangle$ has the minimum value of one whenever $E_{ex} = \ln p$, and it has a maximum 'envelope', resulted by joining the data points at energies $E_{ex} = \ln 2^r$, $r = 1, 2, \ldots$. This implies that the zigzag pattern persists no matter how large the energy is, and that $\langle N_{ex}\rangle$ lies between the range of unity and the envelope.

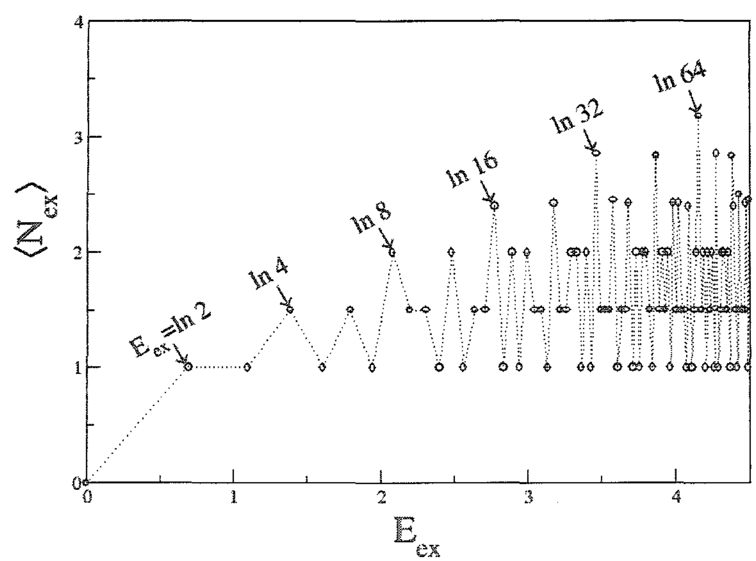


Figure 4.10: Plot of the average bosonic occupancy in the excited states $\langle N_{ex}\rangle$ as function of $E_{ex} = \ln\ n$, where n is an integer. The single-particle energy spectrum is given by $\epsilon_n = \ln\ n$. Note the zigzag pattern, which is similar to Fig. 4.3. The energies $E_{ex} = r \ln 2$ are also indicated.

Note that $E_{ex} = \ln 2^r$ may also be written as $E_{ex} = r \ln 2$. For these values of E_{ex} the problem is the same as that of a one-dimensional harmonic oscillator with the energy spectrum in unit of ($\ln 2\ \hbar\omega$). Thus $\Omega(r \ln 2, N)$ is the same as the number of partitions of

r into N_{ex}, $N_{ex} = 1, 2, \ldots, N$ parts. This can be clearly seen from the many-body partition function, calculated for a few energies (assuming $N \to \infty$):

$$\begin{aligned} Z_N(\beta) \quad = \quad & 1 + \mathbf{x}^{\ln 2} + x^{\ln 3} + \mathbf{2x}^{2\ln 2} + x^{\ln 5} + 2x^{\ln 6} + x^{\ln 7} + \mathbf{3x}^{3\ln 2} + 2x^{\ln 9} + 2x^{\ln 10} \\ & + x^{\ln 11} + 4x^{\ln 12} + x^{\ln 13} + 2x^{\ln 14} + 2x^{\ln 15} + \mathbf{5x}^{4\ln 2} + x^{\ln 17} + 4x^{\ln 18} + x^{\ln 19} \\ & + 4x^{\ln 20} + \cdots + \mathbf{7x}^{5\ln 2} + \cdots + \mathbf{11x}^{6\ln 2} + \ldots, \end{aligned}$$

where, as usual $x = e^{-\beta}$. The coefficients (in bold face) of $x^{r\ln 2}$ are indeed the same as those of a one-dimensional harmonic spectrum, whose partition function is

$$Z_N(\beta) = \prod_{n=1}^{\infty} \frac{1}{1 - x^n} = 1 + x + 2x^2 + 3x^3 + 5x^4 + 7x^5 + 11x^6 + 15x^7 + 22x^8 \ldots.$$

In fact, the $E_n = \ln n$ spectrum might be thought of containing, amongst others, many harmonic-like spectra in units of ($\ln p\ \hbar\omega$), where p is prime. One thus expects the next 'envelope' is given by joining the data points at energies $E_{ex} = r\ln 3$. From Fig. 4.10, it can be seen that this is indeed the case.

The above discussion on $\langle N_{ex}\rangle$ holds also for the microcanonical relative number fluctuation from the ground state, $\langle \triangle N_0\rangle / N$, as shown in Fig. 4.11, where we take $N = 100$. The fluctuation $\langle \triangle N_0\rangle / N$ is minimum and is equal to zero whenever the energy is $\ln p$, since there is only one unique way of exciting N_{ex} ($= 1$) particles at these energies. As in the $\langle N_{ex}\rangle$ case, it also has a maximum envelope below which lie all the other data points. Since there exist infinitely many primes, $\langle \triangle N_0\rangle / N$ oscillates between zero and the envelope and thus remains non-smooth for large energy, similar to the $\langle N_{ex}\rangle$ case. Therefore, even though the microcanonical number fluctuation in this case is non-zero, it

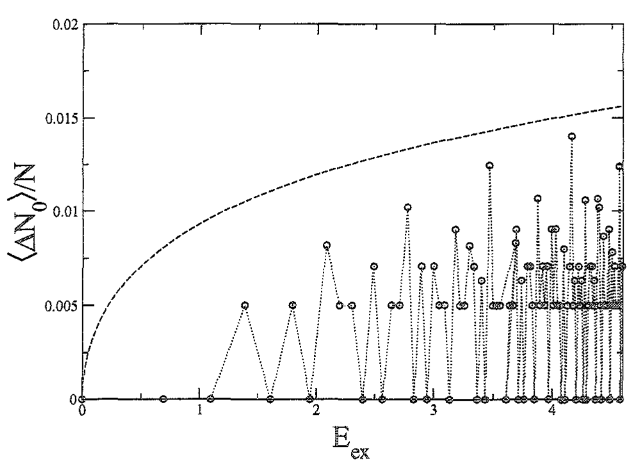


Figure 4.11: The microcanonical relative number fluctuation from the ground state for the same single-particle energy spectrum as in Fig. 4.10. The number of particles is taken as $N = 100$. The corresponding canonical curve (dashed line) is also shown for comparison.

still does not agree with the canonical one, no matter how large N and E are. While the zigzag pattern of the microcanonical number fluctuation always persists, the canonical curve is smooth for all energies, as shown by the dashed curve in Fig. 4.11. A comparison between the exact relative number in the excited states with its canonical counterpart is similar to the one shown in Fig. 4.6 and is therefore not shown.

It is clear that the $\ln n$ spectrum has similar pathological properties as the $\ln p$ spectrum. In the $\ln p$ case, it is recognized that the pathology stems from the fact that there is a one-to-one correspondence between the microstate and the macrostate. In this case, however, the use of the CE or the GCE is still invalid even though there is not a one-to-one correspondence. Instead, the source of the pathology here is the intrinsic oscillation of the many-body multiplicity of states $\Omega(E, N)$, which varies from unity when the many-body $E_n = \ln p$ to some value which can be very large when $E_n = r \ln 2$. This oscillation gets progressively larger when the energy is increased. Since the microcanonical entropy is given by the logarithm of the multiplicity $\Omega(E, N)$, it too has the same peculiar behavior.

4.3 The Microcanonical Entropy

In this section, we focus our discussion more on a different thermodynamics quantity, namely the entropy, rather than the number fluctuation. In a mean-field model, or a model in which the particles are noninteracting, one is generally given a set of single-particle quantum spectrum. From this, a set of many-body eigenenergy is constructed (see section 2.2.1) and the many-body degeneracy factor $\Omega(E, N)$ is determined. The microcanonical entropy of such system is then given by Eq. (2.27):

$$S_N(E) = \ln \Omega(E, N).$$

We have seen, however, that finding the exact degeneracy $\Omega(E, N)$ is not an easy task, especially for large energy. Consequently one generally resorts to the CE, or the GCE. The exact microcanonical entropy is desired, however, for systems which are totally isolated. Since the canonical entropy differs from the microcanonical one due to thermal fluctuation, efforts have been made to find ways to correct for this, especially in the discipline of black hole physics [39, 40, 72, 41] (assuming quantum fluctuation is small). It is not our intention to discuss black hole physics here, however. Rather, our approach is general, and applies for any system where a many-body eigenenergy spectrum is known. For a given many-body eigenenergy spectrum, we derive a formula to approximate the microcanonical entropy. This has already been done in Ref. [39]. However, the formula has not been explicitly tested. This is done here for several models, where the microcanonical entropies may be determined exactly.

4.3.1 Correction to the canonical entropy

Consider a many-body quantum system with eigenenergies E_n that are completely specified by a single quantum number n,

$$E_n = f(n), \; n = 0, 1, 2, \ldots, \tag{4.32}$$

where we assume $f(n)$ to be an arbitrary monotonous function with a differentiable inverse, $f^{-1} = F(x)$, such that $n = F(E_n)$. We know from chapter 2, section 2.2.2 that the multiplicity of states and the smooth part of the density of states of such system are related by (Eq. (2.33)):

$$\bar{\rho}_N(E) = \Omega(E, N)|F'(E)|,$$

where the oscillating part of the density of states has been neglected. The microcanonical entropy is thus given by

$$\begin{aligned} \mathcal{S}_N(E) &= \ln \Omega(E, N) \\ &\sim \ln \bar{\rho}_N(E) - \ln |F'(E)|. \end{aligned} \tag{4.33}$$

The next step is to find $\bar{\rho}_N(E)$. This has already been shown in section 2.2.2 using the canonical partition function $Z_N(\beta)$ (Eq. (2.34)):

$$\bar{\rho}_N(E) = \frac{e^{S_N(\beta_0)}}{\sqrt{2\pi S_N''(\beta_0)}},$$

where $S_N(\beta_0)$ is the canonical entropy evaluated at the equilibrium inverse temperature β_0. The final expression for the microcanonical entropy is thus:

$$\mathcal{S}_N(E) \sim S_N(\beta_0) - \frac{1}{2} \ln \; 2\pi S_N''(\beta_0) - \ln |F'(E)|. \tag{4.34}$$

The energy and the equilibrium inverse temperature are related by

$$E = \langle E \rangle = -\left(\frac{\partial \ln Z_N(\beta)}{\partial \beta}\right)_{\beta_0}. \tag{4.35}$$

Note that the second derivative of the function $S_N(\beta) = \beta E + \ln Z_N(\beta)$ is given by

$$\begin{aligned} S_N''(\beta) &= \frac{\partial^2}{\partial \beta^2} \ln Z_N(\beta), \\ &= \frac{1}{Z_N(\beta)} \frac{\partial^2 Z_N(\beta)}{\partial \beta^2} - \left(\frac{1}{Z_N(\beta)} \frac{\partial Z_N(\beta)}{\partial \beta} \right)^2, \\ &= \langle E^2 \rangle - \langle E \rangle^2, \end{aligned} \tag{4.36}$$

Therefore, $S_N''(\beta_0)$ is the thermal fluctuation squared of energy from the equilibrium. Thus, ignoring the $\ln|F'(E)|$ for now, the microcanonical entropy may be obtained from the canonical one with the energy fluctuation subtracted out, both evaluated at the equilibrium temperature. We shall see that whether the $\ln|F'(E)|$ term contributes depends on the nature of the single-particle energy spectrum.

The approximation (4.34) for the microcanonical entropy $\mathcal{S}_N(E)$ is useful since it is prohibitively difficult to calculate it directly from Eq. (2.27). Generally, in a mean-field model, a single-particle quantum spectrum is obtained. As we have seen from previous chapter, the direct computation of the many-body degeneracy factor $\Omega(E, N)$ from this starting point is very time consuming. Instead, it is much simpler to obtain the canonical many-body partition function and then compute the canonical entropy $S(\beta_0)$. Going one step further, one may calculate the canonical energy fluctuation, and use Eq. (4.34) to obtain $\mathcal{S}_N(E)$. By following this canonical route, no computation of $\Omega(E, N)$ is necessary. We now test the formula for three models, where the exact entropies can be determined. In the first model considered, the system consists of N bosons in a power-law single-particle spectrum. In the second, N distinguishable particles in a d-dimensional harmonic energy spectrum. Finally, we consider N bosons in the $\ln p$ spectrum in the last model.

4.3.2 The power-law single-particle spectrum

For our first model, we consider N noninteracting bosons confined in a mean field with a single-particle spectrum given by $\epsilon_m = m^s$, where the integer $m > 0$, and $s > 0$. This model is considered here because of its connection to number partition theory which makes analytical work possible (see chapter 3). The N-body canonical partition function is given by the generating function for $\Omega(E, N)$ and is exactly known. We shall let $N \to \infty$ in this model and omit the 'N' in the notation. The microcanonical entropy is found by taking the logarithm of $\Omega(E)$, which is determined by expanding its generating function, given by

$$Z(x) = \prod_{m=1}^{\infty} \frac{1}{1 - x^{m^s}}$$

(table 2.1, also see Eq. (3.2)), in series of x. Recall from chapter 3 that for the single-particle power-law eigenenergy spectrum, $|F'(E)| = 1$. Thus this term does not contribute to the RHS of Eq. (4.34). The canonical entropy and its second derivative, as functions of energy E are given by Eqs. (3.9) and (3.10):

$$\begin{aligned} S(\beta_0) &= (1+s)\kappa_s E^{1/(1+s)} + \frac{1}{2}\ln\kappa_s - \frac{s}{2(1+s)}\ln E - \frac{s}{2}\ln 2\pi, \\ S''(\beta_0) &= \frac{1+s}{s}\frac{E^{\frac{1+2s}{1+s}}}{\kappa_s}, \end{aligned}$$

where κ_s is a function of s only. The comparison is done for $s = 1, 2$ and is shown in Figs. 4.12 and 4.13. The dashed curve denotes the canonical entropy $S(E)$ without the correction, and the continuous curve the exact microcanonical entropy $\mathcal{S}(E)$ for the two power laws. We see from these curves that the two differ substantially as a function of the excitation energy E, specially for $s = 2$. Inclusion of the logarithmic correction to the canonical entropy using Eq. (4.34) results, however, in almost perfect agreement, as shown by the dot-dashed curves in these figures.

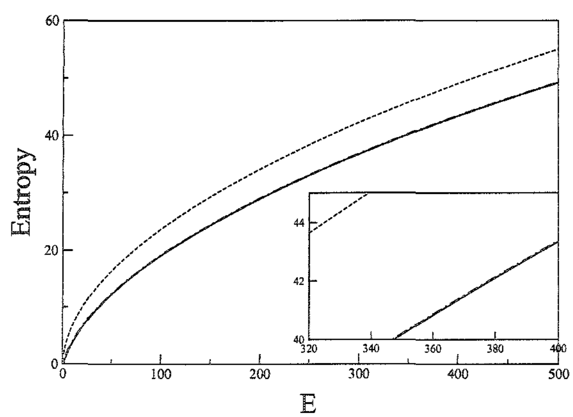


Figure 4.12: Comparison of the exact microcanonical entropy $\mathcal{S}(E)$ (solid line) and the canonical entropy $S(E)$ (dashed line) for the $\epsilon_m = m^s$ spectrum, where $s = 1$. The particles are taken to be N noninteracting bosons, where $N \to \infty$. The dot-dashed curve, given by Eq. (4.34), overlaps with the exact solid curve. The inset shows a zoom-in for $E = 320 - 400$ to reveal how closely the dot-dashed curve follows the exact solid curve.

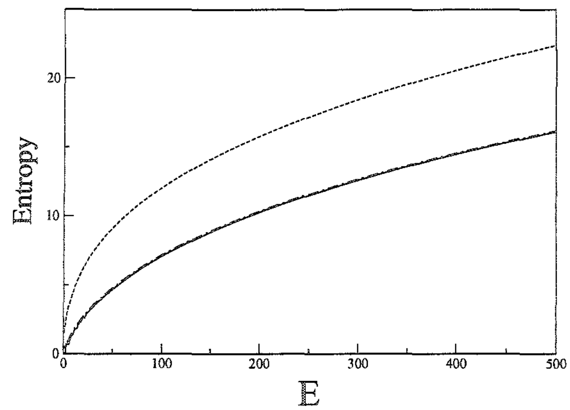


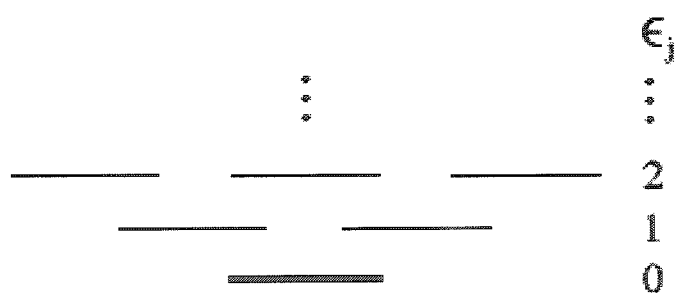
Figure 4.13: Same as in Fig. 4.12, except $s = 2$. The zoom-in is omitted here.

Note that in the exact microcanonical calculation, there is an oscillation due to the discrete nature of $\Omega(E)$. This oscillation is however extremely small and cannot be seen in this scale, except at very low energy. For $s = 1$ (corresponding to the one-dimensional harmonic spectrum), the partition function of noninteracting bosons and fermions are the same, apart from the ground state energy. This means that the degeneracy $\Omega(E)$ and consequently the entropy are the same for both, so that the result shown in Fig. 4.12 applies for fermions also. The same conclusion cannot be made for other values of s since the fermionic partition functions for these cases are not known. For variety we next test the accuracy of Eq. (4.34) for distinguishable particles in d-dimensional harmonic oscillators.

4.3.3 Distinguishable particles in d-dimensional harmonic spectra

To get a feeling of how the counting of states for distinguishable particles differs from that of indistinguishable particles, we work out an example for a few energies explicitly for $d = 1, 2$. A superscript of (1) for one dimension, or (2) for two dimensions, is attached to the ω and Ω to differentiate between the two cases. First, consider a one-dimensional harmonic spectrum. Without loss of generality, we shift the ground state to zero, *i.e.*, $\epsilon_j = j$, $j = 0, 1, 2, \ldots$ in unit of $\hbar\omega$. At zero temperature the N particles are in the ground state. For a given excitation energy, we need to find the number of ways that this energy may be shared amongst these distinguishable particles. For $E_{ex} = 1$, only one particle can get excited, and there are $\binom{N}{1}$ ways of doing this since the particles are all different. Thus

$\omega^{(1)}(1,1,N) = N$, $\omega^{(1)}(1,N_{ex},N) = 0$ for$N_{ex} \neq 1$ and $\Omega^{(1)}(1,N) = N$. For $E_{ex} = 2$, there can be one or two excited particles. Again for one excited particle there are $\binom{N}{1}$ ways and $\omega^{(1)}(2,1,N) = N$. For two there are $\binom{N}{2}$ ways. Thus, $\Omega^{(1)}(2,N) = N + \binom{N}{2} = \frac{N(N+1)}{2}$. For comparison, in the case of boson statistics $\omega^{(1)}(1,1,N) = 1 = \Omega^{(1)}(1,N)$; $\omega^{(1)}(2,1,N) = 1$, $\omega^{(1)}(2,2,N) = 1$, and $\Omega^{(1)}(2,N) = 2$. Consider next the two-dimensional case. Note that in this case there is a degeneracy in the single-particle energy spectrum, given by $g(j) = j + 1$. This degeneracy renders the counting more complicated, as will now be demonstrated for a few excitation energies. The picture below depicts the single-particle energy level of a two-dimensional harmonic oscillator. Each horizontal line represents a state, and the number of lines is the degeneracy $g(j)$. The ground state is singly degenerate, the first excited state is doubly, etc. There are N (distinguishable) particles in the ground state, represented by the thick line.



For $E_{ex} = 1$, there are $\binom{N}{1}$ ways of choosing one particle from the ground state. This particle can then be put either in the 'left' or the 'right' state of the first excited state with $\epsilon_1 = 1$. Thus $\omega^{(2)}(1,1,N) = 2N$ and $\Omega^{(2)}(1,N) = 2N$. Similarly, for $E_{ex} = 2$, $\omega^{(2)}(2,1,N) = 3N$. It is also possible to excite two particles for $E_{ex} = 2$. In this case, there are $\binom{N}{2}$ ways of choosing two particles from the ground state. The two chosen particles, say X and O, may each take one excitation quantum of energy to the first excited level. There are four distinct configurations for this, as shown in the following diagram:

Therefore, $\omega^{(2)}(2,2,N) = 4\binom{N}{2}$, and so $\Omega^{(2)}(2,N) = 3N + 4\binom{N}{2} = \frac{2N(N+1)}{2!}$. Again, for comparison, in the bosonic case $\omega^{(2)}(1,1,N) = 2 = \Omega(2)(1,N)$; $\omega^{(2)}(2,1,N) = 3$, $\omega^{(2)}(2,2,N) = 3$, and $\Omega^{(2)}(2,N) = 6$. The multiplicities in the bosonic case in both dimensions are much less than the distinguishable case. In table 4.3 we show the counting for several values of E_{ex} for one- and two-dimensional harmonic spectra.

E_{ex}	N_{ex}	$\omega^{(1)}(E_{ex},N_{ex},N)$	$\Omega^{(1)}(E_{ex},N)$	$\omega^{(2)}(E_{ex},N_{ex},N)$	$\Omega^{(2)}(E_{ex},N)$
1	1 2 $\vdots$ N	N 0 $\vdots$ 0	N	$2N$ 0 $\vdots$ 0	$2N$
2	1 2 3 $\vdots$ N	N $\binom{N}{2}$ 0 $\vdots$ 0	$\frac{N(N+1)}{2}$	$3N$ $4\binom{N}{2}$ 0 $\vdots$ 0	$\frac{2N(N+1)}{2!}$
3	1 2 3 4 $\vdots$ N	N $2\binom{N}{2}$ $\binom{N}{3}$ 0 $\vdots$ 0	$\frac{N(N+1)(N+2)}{3!}$	$4N$ $2\times 3\times 2\binom{N}{2}$ $[2+\binom{3}{2}]\binom{N}{3}$ 0 $\vdots$ 0	$\frac{2N(2N+1)(2N+2)}{3!}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
E_{ex}	$\vdots$	$\vdots$	$\frac{N(N+1)...(N+E_{ex}-1)}{E_{ex}!}$	$\vdots$	$\frac{2N(2N+1)...(2N+E_{ex}-1)}{E_{ex}!}$

Table 4.3: Tabulation of the multiplicity of states $\Omega(E_{ex},N)$, where the single-particle spectrum is $\epsilon_j = 0,1,2,....$ The superscript (1) denotes the nondegenerate case, $g(j) = 1$, and (2) the degenerate case, $g(j) = j+1$.

It is obvious that the determination of the microstates for distinguishable particles is even more difficult as the energy is increased. However, the multiplicity which is given by the sum of the microstates at a given energy is simple. By inspection, it can be seen from the table that a general expression for $\Omega^{(d)}(E,N)$ is given by

$$\begin{aligned}\Omega^{(d)}(E,N) &= \frac{dN(dN+1)(dN+2)\ldots(dN+E-1)}{E!},\\ &= \frac{\prod_{i=0}^{E-1}(dN+i)}{E!}.\end{aligned} \tag{4.37}$$

Instead of explicit counting as shown above, the multiplicity may also be easily determined using the partition function. For a d-dimensional harmonic spectrum, the one-body partition function is given by

$$Z_1(x) = \frac{1}{(1-x)^d}, \tag{4.38}$$

where as before, x is identified as $e^{(-\beta)}$ in statistical mechanics. Here, it serves as a mathematical parameter < 1 in the generating function for the multiplicity. The N-body partition function for distinguishable particles reads

$$\begin{aligned}Z_N(x) &= Z_1(x)^N,\\ &= (1-x)^{-dN},\\ &= 1+(dN)x+\frac{dN(dN+1)}{2!}x^2+\frac{dN(dN+1)(dN+2)}{3!}x^3+\ldots,\\ &= \sum\frac{\prod_{i=0}^{r-1}(dN+i)}{r!}x^r,\\ &= \sum\Omega^{(d)}(r,N)x^r.\end{aligned} \tag{4.39}$$

Clearly, the expression for $\Omega^{(d)}(r,N)$ is identical to Eq. (4.37), obtained by direct counting. Unlike the case of bose statistics where the multiplicity $\Omega(E,N)$ is found only by expanding the partition function or by exact counting, here, due to the distinguishability property of the system it is given by an explicit formula. For $d=1$, the multiplicity in this model is much larger than that of bosons in a one-dimensional harmonic trap, since the distinguishability property allows more configurations compared to the indistinguishable case. We expect the same is true for higher dimensions. Fig. 4.14 displays a graph of the exact entropy obtained by taking the logarithm of (4.37) for $d=1$ and $N=500$.

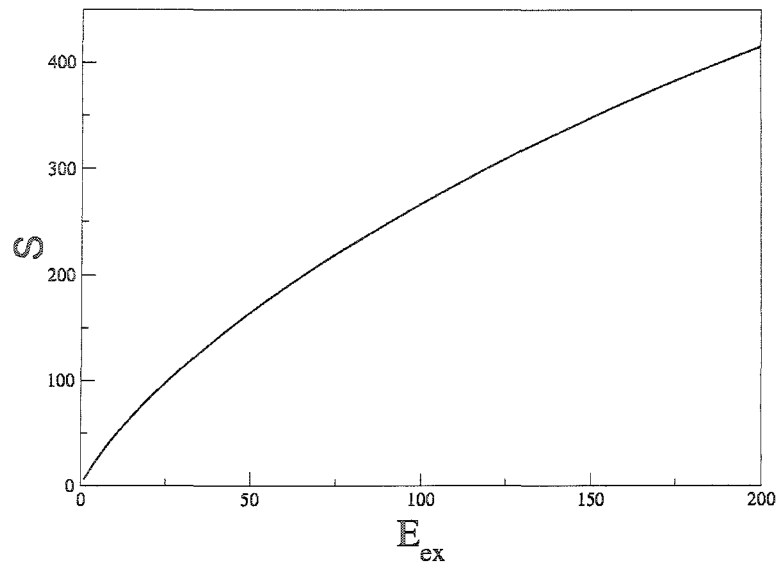


Figure 4.14: Plot of the microcanonical entropy $\mathcal{S}$ for $N = 500$ distinguishable particles. The single-particle energy spectrum is $\epsilon_j = j$, $g(j) = 1$.

We next obtain a the microcanonical entropy in a closed form. Using the Euler-Maclaurin summation formula and the Stirling's series [2](assuming large E and N):

$$
\begin{aligned}
\mathcal{S}_N(E) &= \ln \Omega(E,N) = \sum_{i=0}^{E-1} \ln(dN+i) - \ln E!, \\
&= (dN+E-1/2)\ln(dN+E-1) - E + 1 - dN \ln dN + 1/2 \ln dN + O(\frac{1}{dN}) \\
&\quad -(E+1/2)\ln E + E - 1/2 \ln 2\pi, \\
&\approx E \ln\left(\frac{dN+E}{E}\right) + dN \ln\left(\frac{dN+E}{dN}\right) - \frac{1}{2}\ln\left[2\pi E\left(1+\frac{E}{dN}\right)\right]. \qquad (4.40)
\end{aligned}
$$

We next evaluate the RHS of Eq. (4.34), and see whether it agrees with with Eq. (4.40). Note that as before, the many-body E_n is given by a set of integers, so that $|F'(E)| = 1$. The canonical entropy reads:

$$S_N(\beta) = \beta E - dN \ln(1 - e^{-\beta}). \qquad (4.41)$$

The equilibrium β_0 may be evaluated by setting the first derivative of $S_N(\beta)$ to zero:

$$\beta_0 = \ln\left(\frac{dN}{E} + 1\right). \qquad (4.42)$$

[2] $\ln E! \approx (E+1/2)\ln E - E + 1/2 \ln 2\pi$

Using this β_0, $S_N(E)$ and $S''_N(E)$ can be easily obtained. After some algebraic manipulations, they are given by:

$$\begin{aligned} S_N(E) &= E\ln\left(\frac{dN+E}{E}\right) + dN\ln\left(\frac{dN+E}{dN}\right), \\ S''_N(E) &= E\left(1+\frac{E}{dN}\right). \end{aligned}$$

Putting these in the RHS of (4.34) we obtain:

$$S_N(\beta_0) - \frac{1}{2}\ln\ 2\pi S''_N(\beta_0) = E\ln\left(\frac{dN+E}{E}\right) + dN\ln\left(\frac{dN+E}{dN}\right) - \frac{1}{2}\ln\left[2\pi E\left(1+\frac{E}{dN}\right)\right]$$

which is the same as expression (4.40). Thus, formula (4.34) also works well for distinguishable particles.

4.3.4 The logarithmic spectra

We have seen in section 4.2.1 that the many-body multiplicity of states $\Omega(E) = 1$ for all E. Therefore the microcanonical entropy $S(E)$ is exactly zero for the $\ln p$ single-particle spectrum. The canonical entropy is not zero however, as shown in Fig. 4.15 as a function of temperature T on the left, and excitation energy $\langle E_{ex}\rangle$ on the right. The calculation is done for $N = 100$ bosons for the first 10^6 primes.

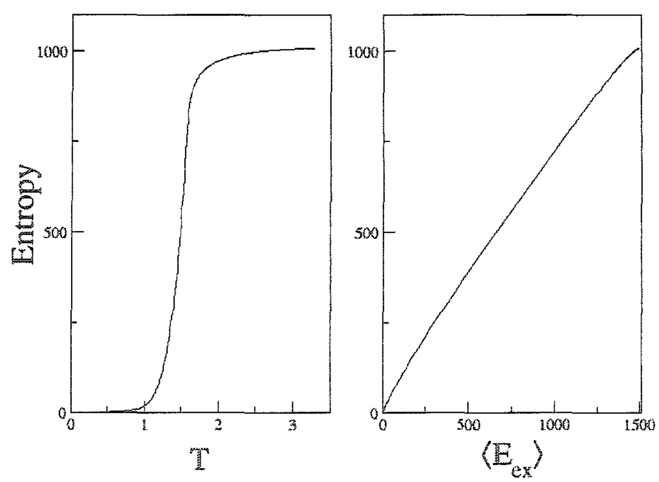


Figure 4.15: Plot of the canonical entropy as a function of temperature T on the left, and excitation energy $\langle E_{ex}\rangle$ on the right, for $N = 100$ bosons. The calculation is done for a truncated spectrum, consisting of first 10^6 primes. The microcanonical entropy is zero.

We next evaluate the RHS of formula (4.34), assuming $N \to \infty$. Recall that the many-body spectrum is given by $E_n = \ln n$, and therefore $n = F(E) = e^E$. Using Eq. (2.32)

$$\rho(E) = \Omega(E)|F'(E)| \left[1 + 2\sum_{k=1}^{\infty} cos\left(2\pi k F(E)\right)\right],$$

the density of states reads

$$\rho(E) = e^E \left[1 + 2\sum_{k=1}^{\infty} cos\left(2\pi k e^E\right)\right]. \tag{4.43}$$

It is important to note that the density of states has an oscillating part, which is the intrinsic quantum fluctuation due to the E_n's taking only discrete values. We now proceed to calculate the canonical entropy. Using the smooth part of $\rho(E)$ in Eq. (2.28), the smooth part of the partition function may be evaluated:

$$\begin{aligned} Z(\beta) &= \int_0^\infty \rho(E) e^{-\beta E} dE, \\ &= \int_0^\infty e^E e^{-\beta E} dE, \\ &= \frac{1}{\beta - 1}. \end{aligned} \tag{4.44}$$

This requires that $\beta > 1$ which is expected. Recall that the exact partition function of this system is known and is given by the Riemann zeta function $Z_N(\beta) = \zeta(\beta)$ which is valid only for $\beta > 1$. Using (4.44), the canonical entropy is thus

$$S(\beta) = \beta E - \ln(\beta - 1).$$

The saddle point, the equilibrium entropy and its second derivative can be easily determined. These are given by:

$$\beta_0 = \frac{1}{E} + 1, \tag{4.45}$$

$$S(E) = E + \ln E + 1, \tag{4.46}$$

$$S''(E) = E^2. \tag{4.47}$$

Putting these in the RHS of (4.34), and using $|F'(E)| = e^E$ we obtain

$$\begin{aligned} S(E) &= E + \ln E + 1 - \frac{1}{2}\ln\left(2\pi E^2\right) - E, \\ &= 1 - \frac{1}{2}\ln 2\pi \approx 0.081, \end{aligned} \tag{4.48}$$

which is independent of E, and the small residue constant is due to the use of the saddle-point method.

We thus see that formula (4.34) applies equally well in this model, where the term $F'(E) \neq 1$. Recall that one peculiar phenomenon of this system is that it is always locked in one microstate, no matter how large the energy is, so that the usual concept of statistical mechanics fails to apply. Therefore, the result found above is rather interesting. For completeness we display a graph of the microcanonical entropy $\mathcal{S}(E)$ in Fig. 4.16 (with $N \to \infty$) for the $\ln n$ spectrum. The entropy is computed exactly by taking the logarithm

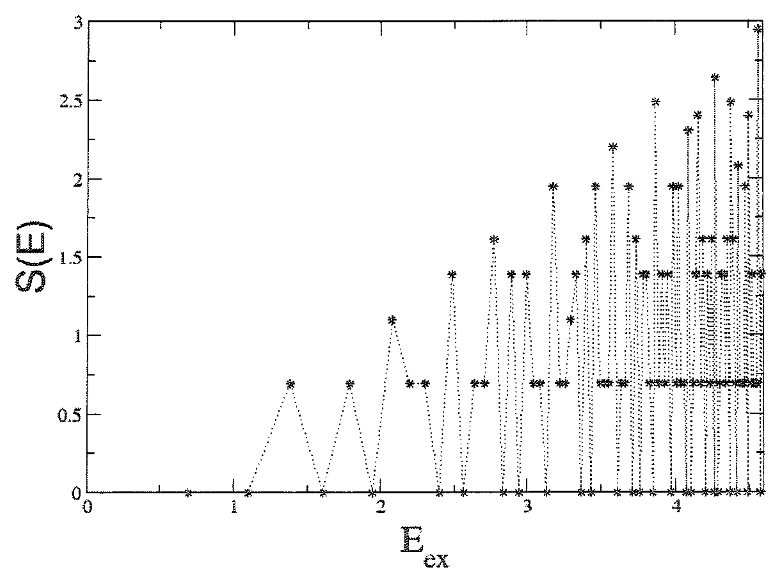


Figure 4.16: Plot of the microcanonical entropy $\mathcal{S}(E)$ for the $\ln n$ single-particle energy spectrum. Note the increasing oscillations as the energy gets larger.

of $\Omega(E)$, tabulated in appendix E for a few energies. Similar to the result for the ground state number fluctuation (Fig. 4.11), the entropy is zero when the energy is $E_n = \ln p$. The oscillation clearly gets larger for larger energy. In this case we cannot test Eq. (4.34) since the many-body density of states is not known, analytical evaluation of the canonical entropy is therefore cannot be done. For comparison, in Fig. 4.17 we show the canonical entropies, obtained numerically, as functions of temperature T and excitation energy for both logarithmic spectra considered. As before we identified the exact excitation energies with the ensemble-averaged $\langle E_{ex} \rangle$. The two results are very similar, with those of the $\ln n$ spectrum larger due to larger number of accessible microstates. These two logarithmic

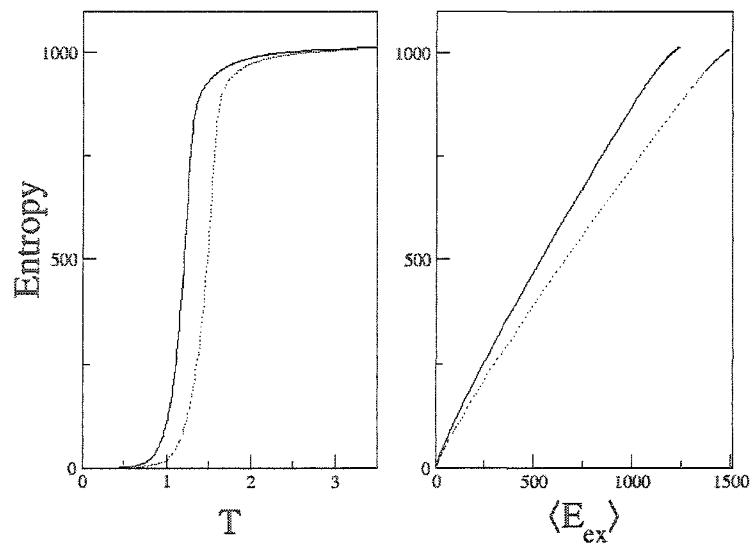


Figure 4.17: Plot of the canonical entropies as functions of temperature T on the left, and excitation energy (E_{ex}) on the right, for $N = 100$ bosons. The calculations are done for truncated spectra, consisting of either first 10^6 integers ($\ln n$ spectrum, solid lines) or primes ($\ln p$ spectrum, dashed lines).

spectra considered, each with its own pathology, provide an interesting counter-example to the principle of thermodynamic equivalence.

We have thus tested formula (4.34) extensively in different models. As mentioned earlier, this formula finds application in black hole physics. It has been used to obtain the leading logarithmic correction to the Bekenstein-Hawking Area Law [39, 40, 72, 41], assuming quantum fluctuation is small. A discussion on the quantum versus thermal fluctuation for the entropy of a black hole can be found in Ref. [72].

Chapter 5

Number Fluctuation of Interacting Trapped Particles

"A complex system that works is invariably found to have evolved from a simple system that works."
John Gaule

In previous chapters we considered several systems in which the (quasi)particles are noninteracting. Recall that the grand canonical divergence of the number fluctuation of ideal bose gas at low temperatures is removed when the more careful canonical or micro-canonical ensembles are used. Within the framework of the conventional grand canonical formalism, the divergence of the particle number fluctuations of a bose gas can be removed by introducing inter-particle interaction [1, 4]. The thermal compressibility χ_T of a gas of density ρ_0 is related to the number fluctuation of the system in the GCE via

$$\frac{(\triangle N)^2}{N} = T\rho_0\chi_T. \tag{5.1}$$

Thus, the compressibility diverges as the fluctuation diverges. The compressibility χ_T is defined in terms of the volume and pressure of the system by

$$\chi_T = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right). \tag{5.2}$$

For $T \to 0$ (or $T \to T_c$ if there is BEC), the pressure is independent of volume, so that $\chi_T \to \infty$ and hence $\triangle N \sim 0(N)$. With interaction, however weak, there is a pressure due to interaction to ensure the fluctuation to be finite. In the case of ideal fermions, there exists a Pauli pressure even though the gas is noninteracting so that the ground state fluctuation is finite (Eq. (2.24)).

Not long after the renewed interest in calculating the number fluctuation of ideal bose gas outside the GCE framework, the question of how interatomic interactions affect the fluctuations of the condensate was examined [20, 22, 73, 21, 23]. Unlike the case of the ideal gas however, the number fluctuation in the presence of interaction is not a well-defined problem. The difficulty arises from the fact that there is no unique way of defining the condensate fraction, and no exact energy spectrum of the interacting system is known. Different methods of approximation for the interacting bose gas yield different results, though they all give finite compressibility. Using the Bogoliubov number nonconserving description at a temperature T, Giorgini *et al.* [20] predicted an anomalous scaling of the fluctuation with the box, $\langle \triangle {N_0}^2 \rangle \sim V^{4/3}$, which ensures that $\langle \triangle {N_0}^2 \rangle / V^2 \sim V^{-2/3} \rightarrow 0$ as $V \rightarrow \infty$. This is different from the grand canonical result which gives $\langle \triangle {N_0}^2 \rangle = N_0(N_0+1) \sim V^2$. However, Idziaszek *et al.* [22] found that $\langle \triangle {N_0}^2 \rangle \sim V$ using the lowest-order perturbation theory and a two-gas model. Soon after, Illuminati *et al.* [21] reached the same conclusion as Idziaszek *et al.*, and also obtained the same formula (4.25) which relates the fluctuations between the MCE and the CE for interacting particles. The authors in these last two references argued that the result of Giorgini *et al.* is questionable due to the number nonconserving method. Using the number conserving operator formalism, however, the prediction of Giorgini *et al.* was supported by Kocharovsky *et al.*. Recently, Xiong *et al.* [23] investigated the problem using both the lowest-order perturbation theory and the Bogoliubov theory within the CE and obtained the same scaling as Giorgini *et al.*. In fact, this anomalous scaling of the particle fluctuation with volume has been shown to be a general property of a Bose condensed system [74].

In this chapter we use exactly solvable interaction models, and examine what happens to the number fluctuations from the ground state as functions of temperature in all three statistical ensembles. In one dimension we consider the inverse square two-body interaction (the Calogero-Sutherland, abbreviated CSM) [75, 76]. This interacting model may be mapped onto the Haldane-Wu generalized exclusion statistics (also known as fractional exclusion statistics, FES) whose quasiparticles are noninteracting, characterized by a parameter g [77, 78, 79, 80, 81, 82, 83, 84, 85]. The value of g represents various degrees of 'Pauli blocking'. Thus, $g = 0, 1$ correspond to free bosons, fermions respectively. The model is solvable, and the quasiparticle energy spectrum is exactly known. In two dimensions we use a self-consistent Thomas-Fermi model for a repulsive zero-range interaction and calculate the number fluctuation in the GCE. This model may also be mapped onto a system of noninteracting particles obeying the Haldane-Wu exclusion statistics. In one dimension our choice of these models has a two-fold advantage. First, it serves as a theoretical tool to demonstrate that the divergence in the GCE is removed when an interaction is introduced, no matter how weak. Second, owing to the mapping to noninteracting FES particles, the model enables us to show that the divergence is removed even for an ideal gas provided that the Pauli blocking is not zero. In the first section, we review the concept of Haldane-Wu's exclusion statistics, whose properties are used in later sections to calculate the ground state number fluctuation of interacting particles.

5.1 Fractional Exclusion Statistics

A way of characterizing the statistics of particles is through their properties under exchange, such as the case of fermions and bosons. Whereas fermions and bosons may exist in all dimensions, certain low dimensional systems have elementary excitations which obey exotic quantum statistics. One example of such system is the celebrated fractional quantum Hall effect (FQHE), where the quasiparticles are anyons [86]. These particles are related to braiding properties of particle trajectories in two spatial dimensions whose many-body wave functions pick up a phase $e^{i\alpha\pi}$ under the exchange of any two particles [87, 88]. The parameter α is called the exchange statistics parameter. Thus $\alpha = 0$ corresponds to completely symmetric wave function, and $\alpha = 1$ antisymmetric. In the first case the particles obey boson statistics, in the second fermion statistics, and anyons are characterized by other arbitrary values of α. The concept of anyons is, however, specific to two dimensions. While studying 'spinons excitations' in one-dimensional antiferromagnets, Haldane [77] was motivated to formulate an alternate definition of fractional statistics which is based on a generalized exclusion principle, and is independent of space dimension. Rather than modifying the many-body exchange phases, this new notion of statistics generalizes the Pauli principle by introducing new rules for occupying single-particle quantum states. The basic idea is that a change in the number of particles, $\triangle N_j$, to a system blocks $\triangle d_i$ of the states available for the next particle. Assuming that the relation is linear, Haldane defines the *statistical interaction* via

$$g_{ij} = -\frac{\triangle d_i}{\triangle N_j}, \tag{5.3}$$

while the size of the system and the boundary conditions are kept fixed, and i, j denote different quantum numbers. Since the numbers of available single-particle states d_i are independent of N_j for bosons, $g_{ij} = 0$. For fermions, they decrease by one for each particle added to the *same state* i, and is unaffected otherwise, $g_{ij} = \delta_{ij}$. Thus Bose and Fermi statistics belong to a class in which statistical interaction operates only between particles in the same state. The CSM also belongs to this class [81, 89, 90]. An example of the more general case where statistical interaction exists between particles of distinct momenta is the repulsive one-dimensional δ-function Bose gas [91]. In this work we shall consider only the first type of interaction. Eq. (5.3) then simplifies to

$$g = -\frac{\triangle d}{\triangle N}. \tag{5.4}$$

The parameter g is thus a measure of the partial Pauli blocking in the system. This concept is further elaborated in the example shown below. The first column lists the number of particles, which vary from 1 to N. In the next three columns are the corresponding values of d^F, d^g, d^B, the available states for fermions, 'g-ons', and bosons respectively. For instance, for $N = 1$, the available states for all three types of particles are d states. When N is changed from 1 to 2, the number of states available for this second particle in the case of fermions is $d-1$, since one state is already blocked by the first particle (Pauli principle). However, there is no Pauli blocking for bosons so that the number of available states remains equal to d. For 'g-ons', there is a partial Pauli blocking, characterized by g, and the number of available states for this second particle is therefore $d-g$. In general, the remaining number

N	d^F	d^g	d^B
1	d	d	d
2	$d-1$	$d-g$	d
3	$d-2$	$d-2g$	d
$\vdots$	$\vdots$	$\vdots$	$\vdots$
N	$d-(N-1)$	$d-g(N-1)$	d

of available states after N particles have been added to the system is given by

$$d^F = d-(N-1), \tag{5.5}$$

$$d^g = d-g(N-1), \tag{5.6}$$

$$d^B = d = d^F + (N-1). \tag{5.7}$$

Since $\triangle N = 1$, it can be seen from the example that the parameter g is indeed as given by relation (5.4). This definition of statistics is known as the Haldane-Wu statistics [77, 92], or the Fractional Exclusion Statistics (FES) [80, 81]. This new definition was applied by Haldane to the one-dimensional spin chain system, as well as the FQHE system where he showed that the anyons gas confined to the lowest Landau level satisfy FES with $g = \alpha$.

5.2 One-dimensional Model

In chapter 4, section 4.1.2, we encountered an explicit example of fermions to bosons mapping for ideal gas in a one-dimensional harmonic trap. As mentioned before, it is in fact well known that in (1+1) dimensions, fermionic theories may be mapped into bosonic ones and vise versa [63, 64, 65]. It was further realized that there exist several models of interacting particles in one dimension which exhibit a continuous boson-fermion interpolation, when the coupling constant varies in appropriate range. One such model is the well-known CSM, whose particles interact via a two-body inverse square potential. Using the thermodynamic Bethe ansatz [91], it was shown that the statistical interaction in the CSM is purely between particles with identical momenta. These particles are equivalent to free particles obeying FES [78, 81, 83, 93, 94, 95, 96]. The Hamiltonian in the CSM is given by ($\hbar = 1,\ m = 1$) [75, 76, 81]:

$$H = \sum_{i=1}^{N}\left[-\frac{1}{2}\frac{\partial^2}{\partial x_i^2} + \frac{1}{2}\omega^2 x_i^2\right] + \frac{1}{2}\sum_{i<j}^{N}\frac{g(g-1)}{(x_i - x_j)^2}. \tag{5.8}$$

The many-body wave function vanishes as $|x_i - x_j|^g$ whenever particles i and j approach each other. For $g = 0$ and 1, the model describes free bosons and fermions respectively. Obviously, the two solutions to the equation $\lambda = g(g-1)$ given by

$$g = \frac{1}{2} \pm \frac{1}{2}\sqrt{1+4\lambda}$$

with g real require $\lambda \geq -1/4$. These two solutions

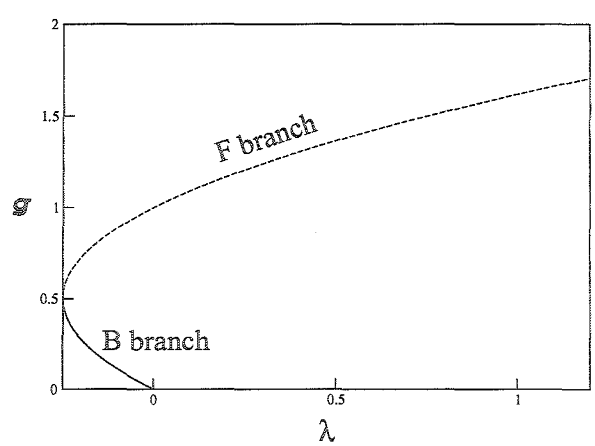


Figure 5.1: Plot of the two branches as described in text. The upper branch (F branch) is for fermions and the lower (B branch) for bosons.

correspond to two branches, as plotted in Fig. 5.1. Since the upper branch contains the noninteracting fermionic value of $g = 1$, this branch is chosen when one works in the fermionic basis, and vice versa for the lower branch. Thus, in the fermionic basis $g \geq 1/2$ while for bosons $0 \leq g \leq 1/2$. Here, we shall assume the particles to be interacting fermions with interacting parameter g. The many-body spectrum reads [76, 81]

$$E\left[\{n_k\}\right] = \sum_{k=1}^{\infty} \epsilon_k n_k - \omega(1-g)\frac{N(N-1)}{2}, \tag{5.9}$$

where $\{n_k\}$ are the (free) fermionic occupancies $= (0,1)$, and $\epsilon_k = (k - \frac{1}{2}\omega)$ denotes the harmonic oscillator energy levels. Although g may not be varied continuously without changing the basis, the energy, as given by Eq. (5.9) is continuous as function of g and is insensitive to the existence of the branches. Therefore, for all practical purpose involving the energy spectrum we may assume that $g \geq 0$. As can be seen from Eq. (5.9), the effect of the interaction is that each particle shifts the energy of every other particle by a constant $\omega(g-1)$. This scale invariant energy shift is the basic reason for the occurrence of nontrivial exclusion statistics [80]. In fact, it is known that quasiparticles with nontrivial exclusion statistics exist in a system that can be solved by the thermodynamic Bethe ansatz [91]. This includes the one-dimensional δ-function gas mentioned earlier, where the statistical interaction operates between particles with different momenta.

The FES single-particle energy level may be obtained by rewriting the energy as

$$E\left[\{n_k\}\right] = \sum_{k=1}^{\infty} \epsilon_k n_k - \omega(1-g)\sum_{i<j=1}^{\infty} n_i n_j, \tag{5.10}$$

where we have replaced $N(N-1)/2$ by $\sum_{i<j=1}^{\infty} n_i n_j$. That these two are equal can be easily shown:

$$\begin{aligned}
\sum_{i<j=1}^{\infty} n_i n_j &= \frac{1}{2}\sum_{i\neq j=1}^{\infty} n_i n_j, \\
&= \frac{1}{2}\sum_i n_i \left[\sum_j n_j - n_i\right], \\
&= \frac{1}{2}\sum_i n_i \left[N - n_i\right], \\
&= \frac{1}{2}\left[N\sum_i n_i - \sum_i n_i^2\right], \\
&= \frac{N(N-1)}{2}.
\end{aligned}$$

To this end, we define

$$\epsilon_g = \epsilon_k - \omega(1-g)N_k, \tag{5.11}$$

where $N_k = \sum_l^{k-1} n_l$ denotes the number of particles *below* energy level k. Eq. (5.11) is nothing but the FES single-particle energy since the total energy (5.10) can now be written as

$$E\left[\{n_k\}\right] = \sum_{k=1}^{\infty} \epsilon_g n_k. \tag{5.12}$$

Using Eq. (5.11), one may determine the spectra of FES particles for any value of g. In Fig. (5.2) we show an example of how to find the spectrum of semions ($g = 1/2$) for three values of excitation quanta $E_{ex} = 1, 2, 3$ and number of particles $N = 5$. The 'Fermi level' k_F^g, is defined at zero excitation, with $k_F = N$ for fermions. Starting from the fermionic spectrum on the left, for each value of E_{ex}, the spectrum of semions is drawn and the resulting particles which are in the excited states are determined. In the case of $E_{ex} = 3$, for instance, the only possibility for fermions is to excite one particle and there are 3 ways of doing this as shown. Therefore, $\omega^F(3,1,5) = 3$, and $\omega^F(3,2,5) = \omega^F(3,3,5) = 0$ since 3 quanta are too few to excite 2 or more particles. For semions, however, $\omega^S(3,1,5) = 1$, $\omega^S(3,2,5) = 2$, and $\omega^S(3,3,5) = 0$. Note that $\Omega(3,5) = 3$ in both cases.

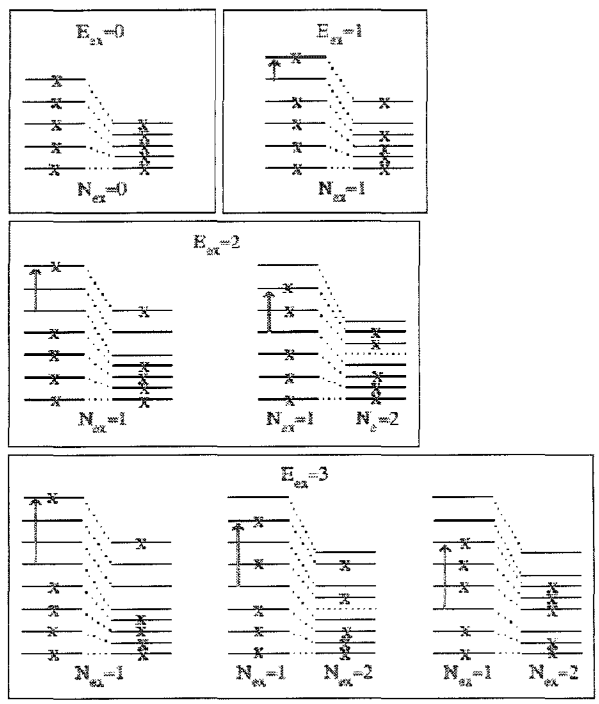


Figure 5.2: Spectra of semions ($g = 1/2$) derived from those of fermions using Eq. (5.11). The (quantum mechanical) ground state is defined at $E_{ex} = 0$. The spectra for different energies are separated by boxes. Within a box there may be more than one configuration, each of which contains the spectrum of ideal fermions on the left and semions on the right. The number of excited particles, N_{ex}, are indicated in each case. The dotted lines are to guide the eye, showing the flow of energy levels from fermions to semions.

5.2.1 Fluctuations in the MCE

We have seen that the energy spectrum of the interacting particles in the CSM or equivalently, of ideal FES particles, are given by those of free particles (fermions or bosons) plus an energy shift that is g dependent. The canonical partition function of these particles thus reads

$$\begin{aligned} Z_N(x) &= x^{E_N^g(0)} \prod_{j=1}^{N} \frac{1}{(1-x^j)}, \\ &= x^{E_N^g(0)} \sum_{n=0}^{\infty} \Omega(n,N) x^n, \end{aligned} \tag{5.13}$$

where, as before, we identify $E = n$, where n is integer. Note that the multiplicity $\Omega(n, N)$ is still the same for FES particles as for bosons and fermions, as already verified by the example shown in Fig. 5.2. The only effect of the interaction strength g is to alter the overall ground state energy $E_N^g(0) = gN(N-1)/2 + N/2$ which reduces to that of fermions, bosons for $g = 1, 0$ respectively. As with bosons or fermions, the counting method gets more cumbersome for larger values of n and N. Ideally, one wishes to be able to determine $\omega^g(n, N_{ex}, N)$ from $\omega^F(n, N_{ex}, N)$ or $\omega^B(n, N_{ex}, N)$, or from $\Omega(n, N_{ex})$ similar to Eqs. (4.1) and (4.13). This general formula for $\omega^g(n, N_{ex}, N)$ for any g, if it exists, is yet to be found. Here, we present the formulae of the microcanonical multiplicities for only two values of g [30]: $g = \frac{N-2}{N-1}$ (close to fermions), and $g = \frac{1}{N-1}$ (close to bosons). Both of these are found empirically. For $g = \frac{N-2}{N-1}$, $\omega^{\frac{N-2}{N-1}}(n, N_{ex}, N)$ is found to be given by:

$$\omega^{\frac{N-2}{N-1}}(n, N_{ex}, N) = \omega^F(n+N, N_{ex}, N) - \omega^F(n+N, N_{ex}, N-1), \tag{5.14}$$

For $g = \frac{1}{N-1}$:

$$\begin{aligned} \omega^{\frac{1}{N-1}}(n, N_{ex}, N) &= \omega^B(n, N_{ex}, N), \qquad\qquad N_{ex} \neq N-1, N \\ \omega^{\frac{1}{N-1}}(n, N-1, N) &= \omega^B(n, N-1, N) + \omega^B(n-1, N-1, N), \\ \omega^{\frac{1}{N-1}}(n, N, N) &= \omega^B(n-N, N, N). \end{aligned} \tag{5.15}$$

These multiplicities must, of course, satisfy

$$\Omega(n, N) = \sum_{N_{ex}=1}^{N} \omega^g(n, N_{ex}, N). \tag{5.16}$$

For $N \leq 5$ and $n \leq 16$, the values found using Eq. (5.14)-(5.15) were verified with those found using the direct combinatorial method. Using Eqs. (2.3), (2.4), and (2.7), we calculated the exact ground state number fluctuations of interacting particles in the CSM, or equivalently, ideal particles obeying FES. In Fig. 5.3 we display the fluctuations for $N = 5$, $g = 3/4, 1/4$. For comparison we also show the fluctuations of free fermions and bosons. The values for $g = 3/4, 1/4$ obtained using the direct combinatorial method for $n \leq 16$ are also shown in the inset. Note that the curves agree with these values exactly. Note also that the number fluctuations for free fermions and free bosons cross at a certain energy, with the fermionic one starting from smaller at small quanta, to larger at high quanta. This is because the number of possibilities of creating holes within the fermi sea and distributing particles above, which starts from low at small energy, increases more rapidly than for bosons whose ground state consists of only one level. Similar behaviours are observed for FES particles, whose g values ($g = 3/4, 1/4$) represent partial Pauli blocking which are both less than that of fermions. Eqs. (5.14) and (5.15) in principle may be applied for any N. However, since they involve the addition of two quantities which may be very large at large quanta and number of particles, there is a difficulty in obtaining their values accurately. Therefore, without loss of accuracy, we restricted the calculations to $N = 10$. Fig. 5.4 shows the ground state number fluctuation for $N = 10$, $g = 1, 8/9, 1/9, 0$. Note that the curve for $g = 8/9$ ($N = 10$) is closer to that of fermions than for $g = 3/4$ ($N = 5$). Similarly, the curve for $g = 1/9$ is closer to that of bosons than for $g = 1/4$. As N gets larger we expect the fluctuation graphs for $g = \frac{N-2}{N-1}$ to come very close to those of free fermions and $\frac{1}{N-1}$ to free bosons. The formulae (5.14) and (5.15) are therefore useful only for systems with a small number of particles. Other point to note is that in both graphs, the results for $g = \frac{N-2}{N-1}$ are closer to those of fermions than for $g = \frac{1}{N-1}$ to bosons. This can be understood from comparing Eqs. (5.14) and (5.15). Eq. (5.14) involves the *difference* of the fermionic microcanonical multiplicities of two system sizes, whose values may be very similar especially at low quanta. Eq. (5.15), however, involves the *addition* of two bosonic microcanonical multiplicities. This brings the microcanonical multiplicities of $g = \frac{1}{N-1}$ further from those of bosons than $g = \frac{N-2}{N-1}$ from those of fermions.

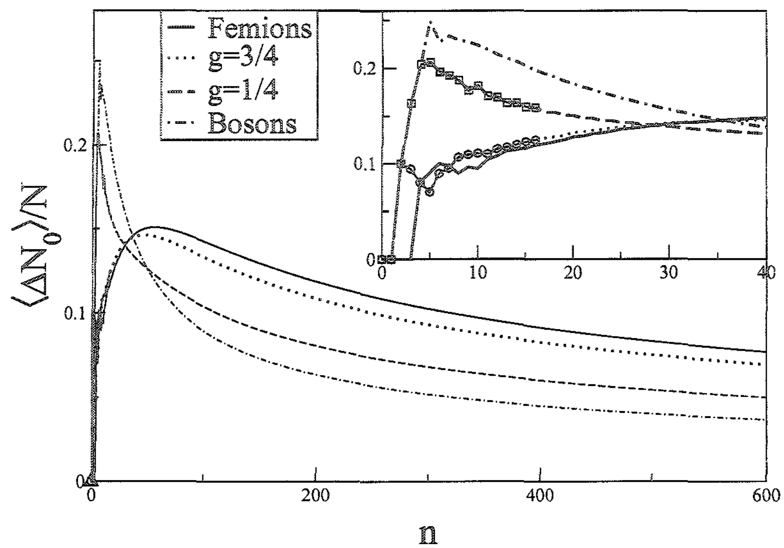


Figure 5.3: Plots of the ground state number fluctuation in the MCE as functions of excitation quanta n for $N = 5$, $g = 1, 3/4, 1/4, 0$. For clarity the low energy part is shown in the inset. The data represented by the symbols are obtained using the direct combinatorial method as shown in Fig. 5.2; ○ for $g = 3/4$, and □ for $g = 1/4$.

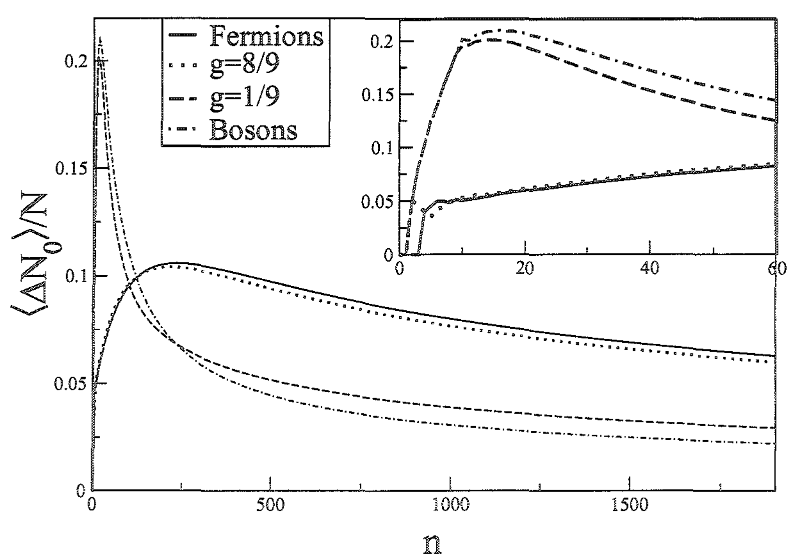


Figure 5.4: Same as Fig. 5.3, except $N = 10$ and $g = 1, 8/9, 1/9, 0$. Unlike Fig. 5.3, however, there is no data from the direct counting in this case.

Although a general formula for the microcanonical multiplicities for any g has not been found, an important point concerning them is observed. For a given number of particles N, consider a set of discrete values of g,

$$g = 1, \frac{N-2}{N-1}, \frac{N-3}{N-1}, ..., \frac{1}{N-1}, 0. \tag{5.17}$$

Since the levels of the FES particles are shifted by an amount which depends on the value of g and the number of particles below (see Eq. (5.11)), for some values of g a particle might lie very close to the 'Fermi level' k_F^g. However, the particles are considered excited if and only if they lie *above* k_F^g, no matter how close. This results in the multiplicities $\omega^g(n, N_{ex}, N)$, for $\frac{N-i}{N-1} > g \geq \frac{N-(i+1)}{N-1}, i = 1, ..., N-1$ *to be the same.* Note the equal sign in $g \geq \frac{N-(i+1)}{N-1}$. For instance,

$$For\ \frac{1}{N-1} > g \geq 0, \qquad \omega^{\{g\}}(n, N_{ex}, N) = \omega^{\{B\}}(n, N_{ex}, N).$$

Note that for these values of g given by Eq. (5.17), the 'Fermi level' $k_F^g = N-(1-g)(N-1)$ is integral. So for $g = (N-j)/(N-1)$, where j is an integer, the 'Fermi level' lines up with the $(j-1)^{th}$ level below k_F of fermions. In the top left box ($E_{ex} = 0$) of Fig. 5.2, for instance, where $N = 5$ and $g = 2/4$ ($j = 3$), the 'Fermi level' lines up with the second level below k_F. This explains why the microcanonical multiplicities for some range of g such that the 'Fermi level' lies between the j^{th} and $(j+1)^{th}$ levels of fermions are the same. This is a consequence of the discrete nature of the energy levels.

5.2.2 Fluctuations in the CE

Using the energy spectrum in CSM given in Eq. (5.9), the N-particle partition function in this one-dimensional model is given by

$$Z_N^g = e^{\beta\omega(1-g)\frac{N(N-1)}{2}} Z_N^F, \tag{5.18}$$

Z_N^F is the N particle fermionic partition function. Setting $g = 0$, the bosonic partition function is obtained,

$$Z_N^B = e^{\beta\omega\frac{N(N-1)}{2}} Z_N^F. \tag{5.19}$$

To avoid confusion, in this section we shall put brackets around quantities like the partition functions when they are raised to some powers, *e.g.*, Z_N^B denotes the bosonic partition function but $(Z_N^B)^g$ denotes the partition function raised to the power g. From (5.19) we obtain

$$e^{-\beta\omega g\frac{N(N-1)}{2}} = (Z_N^B)^{-g}(Z_N^F)^g. \tag{5.20}$$

Using this and Eq. (5.19), Eq. (5.18) may be rewritten as

$$\begin{aligned} Z_N^g &= e^{-\beta\omega g\frac{N(N-1)}{2}} Z_N^B, \\ &= (Z_N^F)^g (Z_N^B)^{1-g}. \end{aligned} \tag{5.21}$$

The canonical partition function given above is exact and may be used for calculating the thermodynamic properties of the system in the CSM within the canonical ensemble formalism. The moments of the occupation number and the number fluctuation are related to the partition function by (appendix A, Eqs. (A.5), (A.6), and (A.15)):

$$\langle n_k \rangle^g = \frac{1}{Z_N^g} y_k \frac{\partial Z_N^g}{\partial y_k}, \tag{5.22}$$

$$\langle n_k^2 \rangle^g = \frac{1}{Z_N^g} y_k \frac{\partial}{\partial y_k}\left(y_k \frac{\partial Z_N^g}{\partial y_k}\right), \tag{5.23}$$

$$\langle \Delta n_k^2 \rangle^g = y_k \frac{\partial \langle n_k \rangle^g}{\partial y_k}. \tag{5.24}$$

where $y_k = \exp(-\beta\epsilon_k)$. Using Eqs. (5.22) and (5.21), $\langle n_k \rangle^g$ can be expressed in terms of those of fermions and bosons via:

$$\begin{aligned} \langle n_k \rangle^g &= \frac{1}{Z_N^g} y_k \frac{\partial Z_N^g}{\partial y_k}, \\ &= \frac{1}{Z_N^g} y_k \left[g(Z_N^F)^{g-1} \frac{\partial Z_N^F}{\partial y_k} (Z_N^B)^{1-g} + (Z_N^F)^g (1-g)(Z_N^B)^{-g} \frac{\partial Z_N^B}{\partial y_k} \right], \\ &= \frac{1}{Z_N^F}\, g\, y_k \frac{\partial Z_N^F}{\partial y_k} + \frac{1}{Z_N^B}\,(1-g)\, y_k \frac{\partial Z_N^B}{\partial y_k}, \\ &= g \langle n_k \rangle^F + (1-g) \langle n_k \rangle^B. \end{aligned} \tag{5.25}$$

Using Eqs. (5.24) and (5.25), the number fluctuation reads

$$\begin{aligned} \langle \Delta n_k^2 \rangle^g &= y_k \frac{\partial \langle n_k \rangle^g}{\partial y_k}, \\ &= y_k \frac{\partial}{\partial y_k}\left[g \langle n_k \rangle^F + (1-g) \langle n_k \rangle^B \right], \\ &= g \langle \Delta n_k^2 \rangle^F + (1-g) \langle \Delta n_k^2 \rangle^B. \end{aligned} \tag{5.26}$$

Eq. (5.26) gives only the fluctuation in the occupation of a given level k, while the quantity we are seeking is the *ground state* number fluctuation. The latter is formally defined in any ensemble as:

$$\langle \triangle N_0^2 \rangle = \sum_k \langle \triangle n_k^2 \rangle = \sum_k (\langle n_k^2 \rangle - \langle n_k \rangle^2) \qquad (5.27)$$

where the sum k runs over only the levels which are completely occupied at zero temperature. Thus, in an *ab initio* calculation, one would formally sum over the quasiparticle levels which are occupied at $T = 0$ to get $\langle \triangle N_0^2 \rangle^g$. Fig. 5.5 shows the level flow in CSM as a function

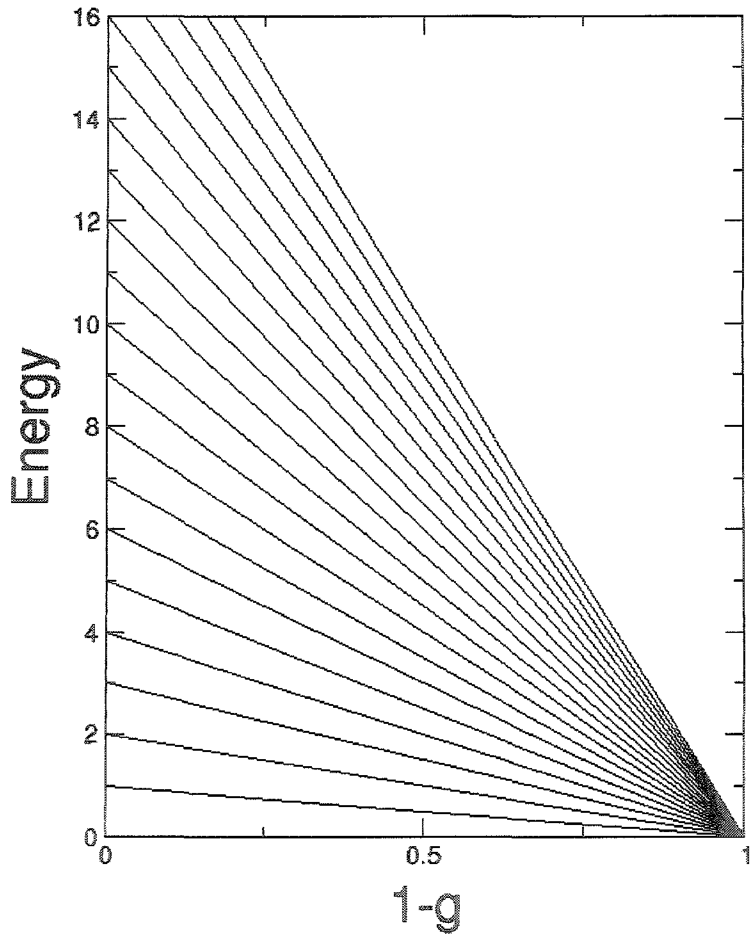


Figure 5.5: The level flow of quasiparticle energy levels in CSM as a function of g

of g obtained from Eq. (5.11) at $T = 0$. It can be seen that as g changes from the fermionic to the bosonic end, the number of levels contributing to the ground state remains constant, while the Fermi energy decreases accordingly. This means that one may obtain $\langle \triangle N_0^2 \rangle^g$ by simply substituting the ground state fluctuations for fermions and bosons, *i.e.*

$$\langle \triangle N_0^2 \rangle^g = g \left\langle \triangle N_0^2 \right\rangle^F + (1-g) \left\langle \triangle N_0^2 \right\rangle^B . \tag{5.28}$$

Thus to find the ground state number fluctuation for FES particles, one needs both those of bosons and fermions.

Given the fact that these are interacting particles in the CSM, Eq. (5.28) is fairly simple. The reason for this is of course due to the mapping of the interacting particles to ideal particles obeying FES. This mapping allows the FES partition function to be expressed in terms of those of fermions and bosons (Eq. (5.18)), which results in the simple expression for the ground state number fluctuation. Note that for $g = 0$ or 1, Eq. (5.28) reduces to that of bosons or fermions respectively. In Figs. 5.6 and 5.7 we compare the microcanonical ground state number fluctuations with the corresponding canonical ones for $g = \frac{N-2}{N-1}, \frac{1}{N-1}$, $N = 5, 10$. In both graphs the microcanonical fluctuations are less than the canonical ones for all excitation energy as expected. Note that the canonical curves for different values of g also cross each other as in the MCE. This property has already been discussed in previous section. The canonical formula (5.28) allows one to calculate the fluctuation for any g. The determination of a general formula for the microcanonical multiplicity, $\omega^g(n, N_{ex}, N)$, and hence the ground state number fluctuation for any g in the MCE, if exists, remains a challenge.

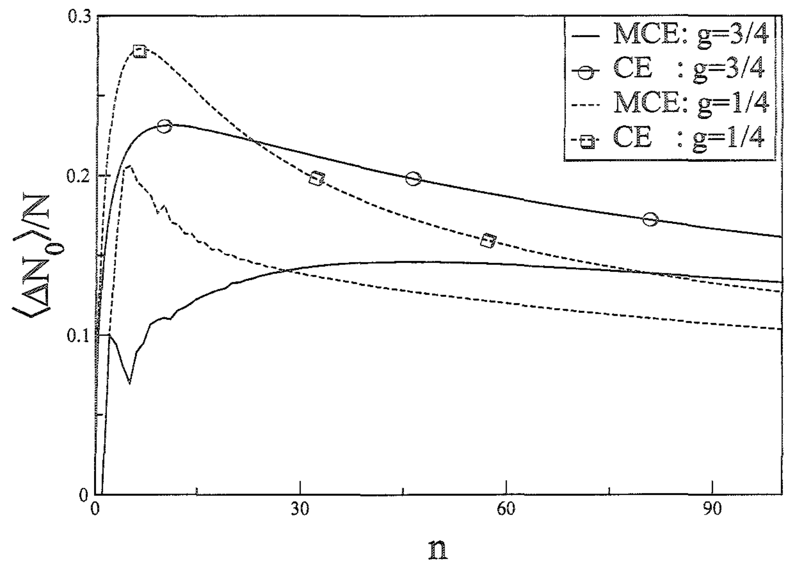


Figure 5.6: Comparison between the microcanonical fluctuations with those in the CE (Eq. (5.28)) for $N = 5$, $g = 3/4, 1/4$.

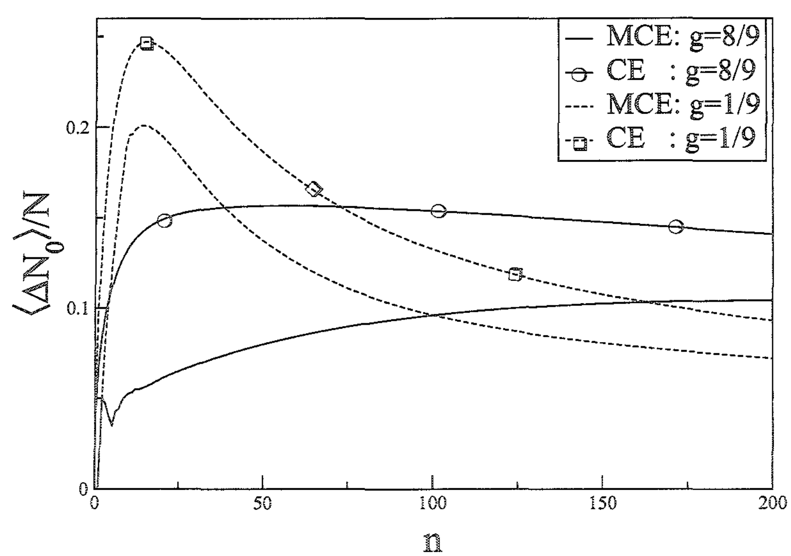


Figure 5.7: Same as in Fig. 5.6, except for $N = 10$, and $g = 8/9, 1/9$.

5.2.3 Fluctuations in the GCE

The thermodynamic properties of an ideal gas of exclusion statistics particles have been widely investigated [29, 92, 97, 98, 99]. While the results in the MCE and CE in previous sections are entirely new, those in the GCE have already been obtained. However, for the sake of completeness we shall discuss them in this section. Specifically, we show the formula for the number fluctuation in the GCE and compare the results obtained here with those from the CE. In the GCE, we point out that the number fluctuation is finite as long as $g \neq 0$.

The distribution function for FES particles reads [92]

$$\langle n_k \rangle = \frac{1}{(w_k + g)}, \tag{5.29}$$

where w_k is the solution of the equation

$$(w_k)^g (1 + w_k)^{1-g} = e^{\beta(\epsilon_k - \mu)}. \tag{5.30}$$

At zero temperature we have,

$$\langle n_k \rangle = \frac{1}{g}, \quad for \;\; \epsilon_k \leq \mu \tag{5.31}$$

and zero otherwise. Note that the distribution function reduces to the usual Fermi and Bose distribution functions Eq. (2.22) for $g = 1$ and $g = 0$ respectively. The distribution function as given above is in fact valid in general and not necessarily restricted to one-dimensional models. However, while it is valid for all temperatures in one dimension, in two dimensions it is valid only for $T > T_c$ in the bosonic basis and thus describes only the non-condensate density. This shall be clarified in the next section, where we discuss the two dimensional case.

The number fluctuation at a given energy ϵ_k is given by

$$\begin{aligned} \langle \triangle n_k^2 \rangle &= \frac{1}{\beta}\frac{\partial \langle n_k \rangle}{\partial \mu}, \\ &= \frac{1}{\beta}\frac{\partial \langle n_k \rangle}{\partial w_k}\frac{\partial w_k}{\partial \mu}. \end{aligned} \tag{5.32}$$

Using Eq. (5.30),

$$\frac{\partial w_k}{\partial \mu} = -\beta \frac{w_k(1 + w_k)}{g + w_k}.$$

Therefore,

$$
\begin{aligned}
\langle \triangle n_k^2 \rangle &= \frac{1}{\beta}\left[-\frac{1}{(w_k+g)^2}\right]\left[-\beta\frac{w_k(1+w_k)}{w_k+g}\right], \\
&= \frac{w_k(1+w_k)}{(w_k+g)^3}, \\
&= w_k(1+w_k)\langle n_k\rangle^3, \\
&= \left[\frac{1}{\langle n_k\rangle}-g\right]\left[\frac{1}{\langle n_k\rangle}+(1-g)\right]\langle n_k\rangle^3, \\
&= [1-g\langle n_k\rangle][1+(1-g)\langle n_k\rangle]\langle n_k\rangle . \qquad (5.33)
\end{aligned}
$$

Eq. (5.33) reduces to Eq. (2.24) for fermions, bosons when $g = 1, 0$ respectively. Thus we have for the number fluctuation from the ground state [29],

$$
\langle \triangle {N_0}^2 \rangle = \sum_k [1-g\langle n_k\rangle][1+(1-g)\langle n_k\rangle]\langle n_k\rangle , \qquad (5.34)
$$

where the sum runs over the levels defining the ground state at $T = 0$. The number fluctuation vanishes at $T \to 0$ since $\langle n_k\rangle \to 1/g$ below the Fermi energy, and zero otherwise. This result holds *no matter how weak* the interaction strength is. However, at $g = 0$, the bosonic limit, the number fluctuation diverges.

In the above we have recourse to the mapping between the CSM and FES and obtained an expression for the number fluctuation at finite temperature. We showed that the fluctuation is finite as $T \to 0$ as long as $g \neq 0$. There is a different approach which makes use of the relationship between the correlation function and number fluctuation [1]. However, this approach works only at $T = 0$ and is not as general. We therefore present the method in appendix F (see also Ref. [24]).

We now compare the ground state number fluctuations obtained in the CE and GCE. Due to numerical difficulty at low temperatures, we are able to do the comparison only for $N = 10$ particles. Despite this limitation, some interesting points can be made. In Fig. 5.8, we show the behavior of the relative ground state fluctuation against temperature of interacting fermions for both ensembles for interacting strengths of $g = 1, 1/2, 0$. In the ideal Haldane-Wu gas picture the $g = 1/2$ case corresponds to semions and the $g = 1$ (0) case is the noninteracting fermionic (bosonic) limit. Note that as $T \to 0$ the GCE fluctuation for free bosons diverges as expected, whereas those for interacting bosons ($g \neq 0$) remain finite and approach zero. The grand canonical fluctuation for semions is found using Eqs. (5.29), (5.30) and (5.34), where μ is determined by the constraint that the average total number of particles is N.

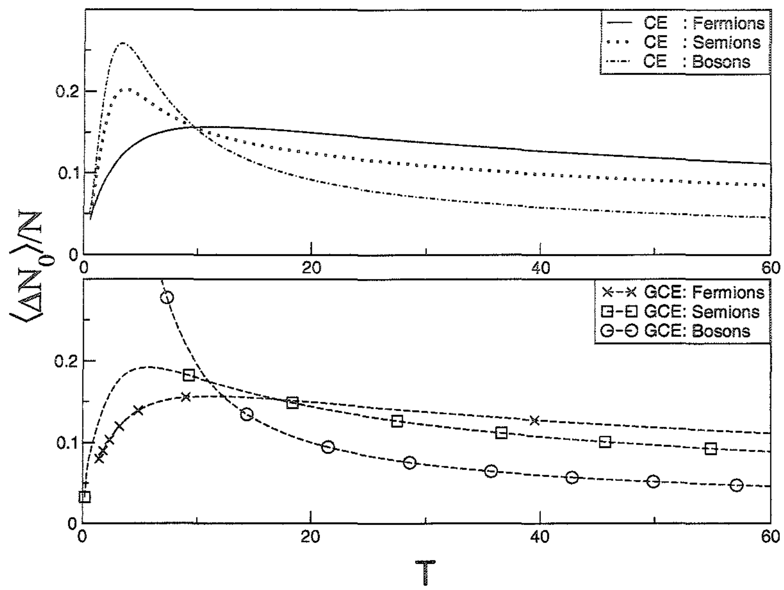


Figure 5.8: The ground state fluctuations for the one-dimensional CSM system in the CE (*Eq.* (5.28)) (top panel) and the GCE (*Eq.* (5.34) (bottom panel) as functions of temperature for $N = 10$. We show the results for fermions, bosons and also semions ($g = 1/2$).

Fig. 5.9 shows the low temperature region of Fig. 5.8. Unlike in the GCE, the canonical ground state fluctuation for free bosons remain finite as $T \to 0$. The ground state fluctuation of free bosons, however, approaches zero *exponentially*, contrary to previous results that found a linear dependence with T all the way to $T = 0$ [9, 26]. In appendix G we give the low temperature expansions of the fluctuation squared $\langle \triangle {N_0}^2 \rangle$ in powers of x, where $x = e^{-\beta\omega}$. At very low temperatures $\langle \triangle {N_0}^2 \rangle$ is independent of the number of particles N (in both GCE and CE). Therefore, the exponential behaviour of the fluctuation of free bosons at low temperatures should remain valid even in the large N limit. In the case of fermions the canonical and grand canonical fluctuations are similar except at very low temperatures. Clearly, the canonical and grand canonical curves of fermions approach zero differently as $T \to 0$. For high temperatures, on the other hand, both ensembles give identical results, as expected.

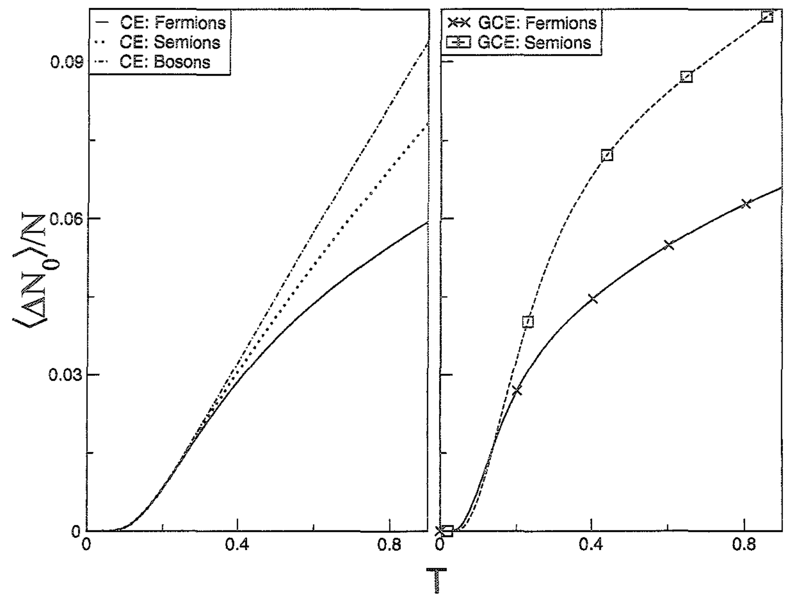


Figure 5.9: Same as in Fig. 5.8 but using the low temperature expansions (see appendix G).

5.3 Two-dimensional Model

While the results in one dimension were derived using the mapping between interacting particles in the CSM to ideal FES particles, extension to higher dimensions is nontrivial since there is no suitable exactly solvable many-body model. However, in the thermodynamic regime, it has been shown that models with short range interactions in two dimension may be regarded as obeying exclusion statistics in the mean-field picture [85, 100, 101]. As mentioned in section 5.2.3, the grand canonical treatment of ideal FES particles applies for all dimensions. In this section, the number fluctuation is derived in the GCE within the mean-field interacting picture. An expression for the number fluctuation is also obtained in the GCE within the noninteracting Haldane-Wu particle picture. These two expressions for the number fluctuation in the two pictures are the same when the interacting strength g in the first picture is identified with the statistical parameter g in the second picture.

5.3.1 Fluctuations in the interacting model

Consider a two-dimensional system of bosons interacting via a zero-range repulsive pseudo-potential. The quantum dynamics is then approximated by the following Hamiltonian

$$H = \sum_{i=1}^{N} \left(\frac{p_i^2}{2m} + \frac{1}{2} m\omega^2 r_i^2 \right) + \frac{\pi\hbar^2}{m} g \sum_{i<j}^{N} \delta(\mathbf{r}_i - \mathbf{r}_j) \ , \tag{5.35}$$

where the momenta and coordinates are planar vectors. This Hamiltonian has been investigated by several groups in connection to atoms in highly anisotropic traps [102, 103, 104, 105]. Using the finite temperature Thomas-Fermi (TF) method [106, 107], it has been shown that the one-body potential generated by the above zero-range interaction, including exchange, is given by

$$U(n(\mathbf{r})) = \frac{2\pi\hbar^2}{m} g n(\mathbf{r}), \tag{5.36}$$

where $n(\mathbf{r})$ is the local number density of the system. It has been observed that the thermodynamic properties of this system have the same form as those of an ideal gas obeying FES [85, 100, 101]. The interaction parameter g in (5.36) plays the role of the statistical parameter, with $g = 0$ for noninteracting bosons. At finite temperature, the TF approximation yields [85, 108]

$$n(\mathbf{r}) = \frac{1}{(2\pi\hbar)^2} \int_0^\infty \frac{d^2p}{\left[\exp[(\frac{p^2}{2m} + V(r) - \mu)\beta] - 1\right]}, \tag{5.37}$$

where

$$V(\mathbf{r}) = \frac{1}{2} m\omega^2 r^2 + \frac{2\pi\hbar^2}{m} g \ n(\mathbf{r}) = V_0(r) + \frac{2\pi\hbar^2}{m} g \ n(\mathbf{r}).$$

It is important to stress that Eq. (5.37) is the non-condensate density, and is equal to the total density only for $T > T_c$. Otherwise the condensate density must be included to give the total density. It was shown in [85, 108] that a self-consistent solution of this equation satisfying $\int n(r) d^2r = N$ may be obtained right down to T=0 for a nonzero positive g. This indicates that the system does not Bose condensate. Accordingly one may take $T_c = 0$ for $g > 0$. However, a condensate solution of this system was recently found using a Hartree-Fock (HF) scheme [109]. Yet when these authors included the presence of phonons in the HF approach (Hartree-Fock-Bogoliubov), they were not able to find BEC solution. These theoretical works are few of the many which contribute to the long-standing debate whether interacting bose gas in two dimensions condensates [109]. In fact, the matter was already settled experimentally when the creation of BEC in a quasi two-dimensional harmonic trap was reported [110]. Adequate theory is yet to be established, however.

In what follows we shall calculate the number fluctuation of the system at finite temperature $T > T_c$. Thus in this section we go a little out of the general theme and consider the total number fluctuation instead of the fluctuation from the ground state. The issue of divergence in the GCE is not dealt with either since Eq. (5.37) does not describe the system at low temperature. Rather, the aim here is to show that the fluctuation in this interacting mean-field model is the same as that of ideal FES model, which shall be determined in the next section.

The momentum integration may be done analytically:

$$n(r) = -\frac{m}{2\pi\hbar^2\beta}\ln\left[1-\exp[-\beta(V(r)-\mu)]\right]. \tag{5.38}$$

The local number fluctuation (between r and $r+dr$) in the GCE is given by

$$\begin{aligned}\langle\triangle N^2\rangle &= \frac{1}{\beta}\frac{\partial n(r)}{\partial\mu}, \\ &= \frac{1}{\beta}\frac{m}{2\pi\hbar^2}\frac{1}{e^{(V(r)-\mu)\beta}-1+g}.\end{aligned} \tag{5.39}$$

The chemical potential μ is a function of temperature, and is determined by the condition that $\int n(r)d^2r = N$ and in the thermodynamic limit it approaches the lowest energy eigenstate as the temperature goes to T_c. The thermodynamic limit is obtained by taking $N \to \infty$ and $\omega \to 0$ such that $N^{1/2}\omega =$ constant. In this limit the local number density becomes a constant and the fluctuation reads

$$\langle\triangle N^2\rangle = \frac{1}{\beta}\frac{m}{2\pi\hbar^2}\frac{1}{\exp[(\frac{2\pi\hbar^2}{m}gn-\mu)\beta]-1+g}, \tag{5.40}$$

We next work in the ideal FES gas picture, and show that the expression for the fluctuation is identical to Eq. (5.40).

5.3.2 Fluctuations in the noninteracting FES model

The local density as a function of the radial coordinate is given by [24],

$$n(\mathbf{r}) = \int \frac{d^2p/(2\pi\hbar)^2}{[w+g]}, \tag{5.41}$$

where the local variable $w(p,r)$ is defined through Wu's equation within TF approximation:

$$(w)^g(1+w)^{1-g} = \exp[\beta(\frac{p^2}{2m}+V_0(r)-\mu)], \tag{5.42}$$

and g is the exclusion statistics parameter which we identify with the interaction strength in the mean-field interacting picture. Using Eq. (5.42),

$$d^2p = \pi d(p^2) = \frac{2\pi m}{\beta}\left(\frac{g}{w}+\frac{1-g}{1+w}\right)dw,$$

and therefore

$$n(r) = \frac{m}{2\pi\hbar^2\beta} \ln\left[\frac{1+w_0}{w_0}\right], \tag{5.43}$$

where the local variable $w_0(r)$ is determined through

$$(w_0)^g(1+w_0)^{1-g} = \exp[\beta(V_0(r)-\mu)]. \tag{5.44}$$

The fluctuation is thus

$$\begin{aligned} \langle \triangle N^2 \rangle &= \frac{1}{\beta}\frac{\partial n(r)}{\partial \mu}, \\ &= \frac{1}{\beta}\frac{m}{2\pi\hbar^2}\frac{1}{w_0+g}. \end{aligned} \tag{5.45}$$

The equivalence between the noninteracting exclusion statistics picture and the mean-field description is established using the following relationship

$$w_0(r) = \exp[\beta(V(r)-\mu)] - 1, \tag{5.46}$$

where $V(r)$ is the self consistent mean-field potential. Substituting this in Eq.(5.45), and taking the thermodynamic limit yields Eq. (5.40). This equivalence allows one to calculate fluctuations in either the mean field picture or in the noninteracting exclusion statistics picture.

Chapter 6

Summary

"The world is round and the place which may seem like the end may also be only the beginning."
Ivy Baker Priest, in Parade, 1958

In this thesis we have investigated a number of problems relating to the number fluctuation from the ground state. Our focus is on problems in which the macrostate or the number fluctuation may be found analytically, mainly by applying the connection to number theory. This can be done more readily for noninteracting particles. For interacting particles, we considered models in which the particles may be thought of ideal, but with modified statistics.

In chapter 2 we review some background theories on how to calculate the number fluctuations in different ensembles, and discuss the many-body multiplicity of states and its relationship with the many-body density of states. Chapter 3 is devoted to the derivation of the different formulae in the theory of number partition using the method of statistical mechanics. Given an energy E, the problem of distributing bosons over the excited states of a one-dimensional harmonic spectrum has been recognized to pertain to integer partitioning. The main quantity is the many-body multiplicity of states, which is identical to the number of partitions of an integer $E = n$. Asymptotic formula for the density of states was obtained for many-body energy spectra given by $E_n = n^s$, where n is integer > 0 and $s > 0$. Using the relationship between the density of states and the multiplicity of states, this asymptotic formula is shown to be equivalent to that of the number of partitions of an integer n into a sum of s^{th} powers of a set of integers $< n$. By considering the particle sector of the fermionic energy spectrum, an asymptotic formula for the number of distinct partitions of n was also obtained. For $s = 1$, using the partition function for finite number of particles N, we derived the Erdos-Lehner formula for the number of restricted partitions of n. Similarly, by imposing a finite particle condition in the pseudo-fermion model, the generating function and the corresponding formula for the number of restricted and distinct partitions of n were derived. This last formula for the number of restricted and distinct partitions of n, to our best knowledge, is new.

In chapter 4, we calculated the number fluctuation from the ground state of noninteracting particles in different traps in the first two sections, and examine a formula for the microcanonical entropy in the last section. In 4.1.1 we review the microcanonical fluctuation for a system of bosons in a one-dimensional harmonic trap. To calculate the number fluctuation from the ground state in the microcanonical ensemble, one needs to find the microstate, which is a function of energy E, number of excited particles N_{ex}, and total number of particles N. The microstate may be determined exactly using an identity in number theory which connects it and the macrostate. Since the macrostate may be determined by expanding the partition function, in principle it suffices to use the identity to calculate the number fluctuation. However, one may go one step further. The macrostate, as previously discussed, is related to the density of states and may be found asymptotically (large E). Thus, for a system of bosons in a one-dimensional harmonic trap, the number fluctuation from the ground state may be analytically calculated. For fermions in the same energy spectrum, discussed in 4.1.2, there is no such analytical formula for the number fluctuation. The difficulty arises from the fact that the fermionic ground state consists of many levels. Although there is no such analytical formula, we have derived an identity relating the microstate and the macrostate similar to that of bosons to calculate the number fluctuation in the MCE for fermions. The identity involves the macrostates of both the particle and hole spaces, and reduces to the formula for bosons when the macrostate for the hole space is set to unity.

The mean occupation number in the ground state is in general thermodynamically equivalent in the GCE and CE, and at high temperature (or energy) to the MCE. The ground state number fluctuation, however, is very sensitive to the ensemble used. In section 4.2 we considered two models in which neither the fluctuation nor the occupation number are thermodynamically equivalent. The single-particle energy spectrum in the first model is given by the logarithm of the prime number sequence, and in the second model the logarithm of the natural number sequence. Consider the first model. The excitation energy is given by the logarithm of an integer n. Since there is no energy fluctuation in the MCE, the problem of distributing the particles over the excited states above zero is equivalent to counting the number of ways that the integer n may be expressed as a product of prime numbers. By applying the fundamental theorem of arithmetic, we showed that the macrostate and the microstate are unity for all excitation energies. As a consequence, the number fluctuation from the ground state is identically zero. Since the system is in equilibrium with a heat bath in the CE, the energy fluctuation is non-zero, with an average energy $\langle E \rangle$, being identified with the excitation energy E_{ex}. The CE thus effectively samples more than one level for a given excitation energy, and consequently the macrostate is greater than unity. This results in a non-vanishing ground state number fluctuation (except at zero excitation or temperature), in contrast to the microcanonical case. For the same reason the mean occupation number is dramatically different in the MCE and the CE, while it is very similar in the CE and the GCE. The number fluctuation in the GCE is, as well known, divergent at low temperature. The result above holds whether the number of particles is finite or very large. Further, it also holds in the case of fermions. The same outcome regarding the differences of the occupation number and the number fluctuation from the ground state in the different ensembles also applies in the second model. Although the single-particle energy spectrum of this model admits more possibilities, the fact that it also contains the $\ln p$ case is the reason for the inequivalence of the ensembles. The excitation energy in this case is also given by the logarithm of n. Whenever n is a prime number, the microstate and the macrostate are the same and equal to one. The fluctuations for these values of the excitation energy vanish in the MCE. Therefore, even though the ground state number fluctuation in the second model does not vanish for all excitations, it oscillates between values of zero and non-zero, while the CE always gives a smooth result.

In the last part of this chapter, section 4.3, we examined a formula which corrects for the thermal fluctuation of the canonical entropy to approximate the microcanonical entropy. In the treatment, the quantum fluctuation is assumed to be small. The microcanonical entropy is by definition given by the logarithm of the macrostate, which in general is very difficult to find. On the other hand, it is much simpler to find the canonical counterpart once the many-body partition function is known. Thus, such formula which approximates the microcanonical entropy is very useful. In this section we tested the accuracy of the formula explicitly for three different models. The merits of these models lie in the fact that their macrostates may be computed exactly. In the first model, we considered N noninteracting bosons in a mean field with a power-law single-particle energy spectrum.

The macrostates of this model have been determined in chapter 3. In the second model, we considered N distinguishable particles in a d-dimensional harmonic spectrum. Due to the distinguishability property of the particles, a formula for the macrostate in this case may be obtained exactly. The last model consists of N bosons in a hypothetical trap with a single-particle energy spectrum given by the logarithm of the prime number sequence. In this special model the macrostate has been shown to be unity for all energy E. In all three cases the approximated formula was found to be in excellent agreement with the exact microcanonical entropy.

Chapter 5 is devoted to the number fluctuation of interacting particles. In one dimension we considered the integrable Calogero-Sutherland model, where the many-body energy spectrum is exactly known. The particles in this model may be looked upon as free and obey the Haldane-Wu statistics, characterized by the statistical parameter g. The microcanonical calculation in this model is difficult. Emperically we obtained the expressions for the microstates and calculated the ground state number fluctuation exactly for only two values of g. In the CE, however, the calculation may be done analytically. An expression for the ground state number fluctuation of these interacting particles was obtained and found to be dependent on both bosonic and fermionic fluctuations. Comparison was made between the results from the different ensembles. The GCE case has been discussed before by different authors but was included here for completeness. In two dimensions we considered a contact interaction. Within the Thomas-Fermi mean-field model we obtained the number fluctuation and showed that it is the same as that of ideal particles obeying Haldane-Wu statistics.

To conclude this thesis, we discuss some problems for future investigation. Due to the equi-spaced and non-degenerate properties, a system of N bosons in a one-dimensional harmonic spectrum pertains to integer partitioning. Since the higher dimensional spectra are also equi-spaced but degenerate, a question arises of whether there is any connection to the theory of number partition. On a similar note, it is interesting to find out whether there exists a connection between number partition and distributing the FES particles over the excited states. We have seen that the statistical parameter $g = 0$ corresponds to the integer partition case, and $g = 1$ (pseudo-fermions) corresponds to the distinct case. Intermediate values of g may result in some form of integer partition. Next, formula (4.34) in section 4.3 which approximates the microcanonical entropy is only for spectra depending on a single quantum number. For it to be applicable in other cases, extension to spectra depending on two or more quantum numbers is needed. Finally, the last problem involves the microcanonical entropy of FES particles. Since there is no known formula nor a method for obtaining the microstate or the macrostate of these particles, the microcanonical entropy cannot be determined. A possible line of research is to use the method of approximating the microcanonical entropy from the canonical counterpart, and extend it for the FES particles. If this is successful, a checking can be done using the exact values for small energies that we obtained by direct counting.

Appendix A

Detailed calculations of Eqs. (2.18) and (2.19)

The N-particle partition function for either bosons or fermions may in general be written in the occupartion number representation as

$$Z_N = \sum_{\{n_l\}} e^{-\beta E_{\{n_l\}}}, \tag{A.1}$$

where n_l is the occupation number of the energy level l, $E_{\{n_l\}}$ is the energy of the N-particle system for a given set of occupancy $\{n_l\}$. For noninteracting particles, the energy of the system $E_{\{n_l\}}$ is given by

$$E_{\{n_l\}} = \sum_l \epsilon_l \; n_l, \tag{A.2}$$

where ϵ_l is the single-particle energy level. For (spinless) fermions $n_l = 0, 1$ and may take any value up to N for bosons. Using Eq. (A.2), Eq. (A.1) may be rewritten as

$$\begin{aligned} Z_N &= \sum_{\{n_l\}} e^{-\beta \sum_l \epsilon_l n_l}, \\ &= \sum_{\{n_l\}} \prod_l e^{-\beta \epsilon_l n_l}, \\ &= \sum_{\{n_l\}} e^{-\beta \epsilon_k n_k} \prod_{l \neq k} e^{-\beta \epsilon_l n_l}, \\ &= \sum_{\{n_l\}} y_k^{n_k} \prod_{l \neq k} e^{-\beta \epsilon_l n_l}, \end{aligned} \tag{A.3}$$

where $y_k \equiv e^{-\beta\epsilon_k}$. Differentiate the above with respect to y_k,

$$\begin{aligned}
\frac{\partial Z_N}{\partial y_k} &= \sum_{\{n_l\}} n_k\, y_k^{n_k-1} \prod_{l\neq k} e^{-\beta\epsilon_l n_l}, \\
&= \sum_{\{n_l\}} \frac{n_k}{y_k} \prod_{l} e^{-\beta\epsilon_l n_l}, \\
&= \sum_{\{n_l\}} \frac{n_k}{y_k} e^{-\beta E_{\{n_l\}}}.
\end{aligned} \tag{A.4}$$

Next, multiply both sides by y_k/Z_N and change the dummy index l to k, we have

$$\frac{y_k}{Z_N}\frac{\partial Z_N}{\partial y_k} = \frac{1}{Z_N}\sum_{\{n_k\}} n_k e^{-\beta E_{\{n_k\}}}.$$

The right hand side of the above is just the definition of the first moment of the occupation number. Therefore,

$$\begin{aligned}
\langle n_k \rangle &= \frac{1}{Z_N}\sum_{\{n_k\}} n_k e^{-\beta E_{\{n_k\}}}, \\
&= \frac{1}{Z_N} y_k \frac{\partial Z_N}{\partial y_k}.
\end{aligned} \tag{A.5}$$

Similarly, the second moment of the occupation number reads

$$\begin{aligned}
\langle n_k^2 \rangle &= \frac{1}{Z_N}\sum_{\{n_k\}} n_k^2 e^{-\beta E_{\{n_k\}}}, \\
&= \frac{1}{Z_N} y_k \frac{\partial}{\partial y_k}\left[y_k \frac{\partial Z_N}{\partial y_k}\right].
\end{aligned} \tag{A.6}$$

It is convenient to express formulae (A.5) and (A.6) in terms of the partition function itself. Using the constraint that $N = \sum_k \langle n_k \rangle$,

$$\begin{aligned}
Z_N N &= Z_N \sum_k \langle n_k \rangle, \\
&= \sum_k y_k \frac{\partial Z_N}{\partial y_k}.
\end{aligned} \tag{A.7}$$

From the recursion relation (2.17) and using $Z_1(j\beta) = \sum_k e^{-j\beta\epsilon_k} = \sum_k y_k^j$,

$$\begin{aligned}
N Z_N &= \sum_{j=1}^{N} (\pm)^{j+1} Z_1(j\beta) Z_{N-j}, \\
&= \sum_{j=1}^{N} (\pm)^{j+1} \sum_k y_k^j Z_{N-j}.
\end{aligned} \tag{A.8}$$

Equating (A.7) and (A.8),

$$y_k \frac{\partial Z_N}{\partial y_k} = \sum_{j=1}^{N} (\pm)^{j+1} y_k^j Z_{N-j}. \tag{A.9}$$

Comparing (A.5) and (A.9), the first moment of the occupation number is simply

$$\langle n_k \rangle = \frac{1}{Z_N} \sum_{j=1}^{N} (\pm)^{j+1} y_k^j Z_{N-j}. \tag{A.10}$$

We next look at the second moment. From (A.6),

$$\begin{aligned}
\langle n_k^2 \rangle &= \frac{1}{Z_N} y_k \frac{\partial}{\partial y_k} \left[y_k \frac{\partial Z_N}{\partial y_k} \right], \\
&= \frac{1}{Z_N} y_k \frac{\partial}{\partial y_k} \left[\sum_{j=1}^{N} (\pm)^{j+1} y_k^j Z_{N-j} \right], \\
&= \frac{1}{Z_N} y_k \sum_{j=1}^{N} (\pm)^{j+1} \left[j y_k^{j-1} Z_{N-j} + y_k^j \frac{\partial}{\partial y_k} Z_{N-j} \right].
\end{aligned} \tag{A.11}$$

Repeating the steps from Eq. (A.7) to Eq. (A.9), it can be seen that

$$y_k \frac{\partial Z_{N-j}}{\partial y_k} = \sum_{i=1}^{N-j} (\pm)^{i+1} y_k^i Z_{N-j-i}. \tag{A.12}$$

Using this in the second term of Eq. (A.11), the second moment of the occupation number is given by

$$
\begin{aligned}
\left\langle n_k^2 \right\rangle &= \frac{1}{Z_N}\sum_{j=1}^{N}(\pm)^{j+1} j y_k^j Z_{N-j} + \frac{1}{Z_N}\sum_{j=1}^{N}\sum_{i=1}^{N-j}(\pm)^{i+j} y_k^{i+j} Z_{N-i-j}, \\
&= \frac{1}{Z_N}\sum_{j=1}^{N}(\pm)^{j+1} j y_k^j Z_{N-j} + \frac{1}{Z_N}\sum_{j=1}^{N}\sum_{l=1+j}^{N}(\pm)^{l} y_k^{l} Z_{N-l}, \\
&= \frac{1}{Z_N}\sum_{j=1}^{N}(\pm)^{j+1} j y_k^j Z_{N-j} + \frac{1}{Z_N}\sum_{l=1}^{N}\sum_{j=1}^{l-1}(\pm)^{l} y_k^{l} Z_{N-l}, \\
&= \frac{1}{Z_N}\sum_{j=1}^{N}(\pm)^{j+1} j y_k^j Z_{N-j} + \frac{1}{Z_N}\sum_{l=1}^{N}(\pm)^{l}(l-1) y_k^{l} Z_{N-l}, \\
&= \frac{1}{Z_N}\sum_{j=1}^{N}(\pm)^{j+1} j y_k^j Z_{N-j} + \frac{1}{Z_N}\sum_{j=1}^{N}(\pm)^{j}(j-1) y_k^{j} Z_{N-j}, \\
&= \frac{1}{Z_N}\sum_{j=1}^{N}(\pm)^{j+1} j y_k^j Z_{N-j} \pm \frac{1}{Z_N}\sum_{j=1}^{N}(\pm)^{j+1}(j-1) y_k^{j} Z_{N-j}, \\
&= \frac{1}{Z_N}\sum_{j=1}^{N}(\pm)^{j+1}\ \left[j \pm (j-1)\right]\ y_k^j Z_{N-j}. \qquad \text{(A.13)}
\end{aligned}
$$

where we have let $l = i + j$ and switched the order of the sums of the second term in the second and third steps. It follows from (A.10) and (A.13) that $\langle n_k \rangle = \left\langle n_k^2 \right\rangle$ for fermions.

The number fluctuation may also be conveniently expressed in terms of the N-particle partition function. Starting from (A.6) and using (A.5),

$$
\begin{aligned}
\left\langle n_k^2 \right\rangle &= \frac{1}{Z_N} y_k \frac{\partial}{\partial y_k}\left[y_k \frac{\partial Z_N}{\partial y_k}\right], \\
&= \frac{1}{Z_N} y_k \frac{\partial}{\partial y_k}\left[\langle n_k \rangle Z_N\right], \\
&= \frac{1}{Z_N} y_k \left[Z_N \frac{\partial \langle n_k \rangle}{\partial y_k} + \langle n_k \rangle \frac{\partial Z_N}{\partial y_k}\right], \\
&= \frac{1}{Z_N} y_k \frac{\partial Z_N}{\partial y_k}\langle n_k \rangle + y_k \frac{\partial \langle n_k \rangle}{\partial y_k}, \\
&= \langle n_k \rangle^2 + y_k \frac{\partial \langle n_k \rangle}{\partial y_k}. \qquad \text{(A.14)}
\end{aligned}
$$

Thus,

$$
\begin{aligned}
(\triangle n_k^2) &= \left\langle n_k^2 \right\rangle - \langle n_k \rangle^2, \\
&= y_k \frac{\partial \langle n_k \rangle}{\partial y_k}. \qquad \text{(A.15)}
\end{aligned}
$$

Appendix B

Detailed calculations of Eq. (2.34)

We start by using

$$S_N(\beta) = \beta E + \ln Z_N,$$

Eq. (2.30) becomes

$$\rho_N(E) = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} Z_N e^{\beta E} d\beta = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} e^{S_N(\beta)} d\beta. \tag{B.1}$$

The integration over the parameter β is along the imaginary axis, and the function $S_N(\beta)$ is complex. This results in the integrand being oscillatory, with most of the contribution coming from a point β_0 on the real axis at which $S_N(\beta)$ is stationary. For a given E, this stationary point may be found from

$$\left(\frac{\partial S_N(\beta)}{\partial \beta}\right)_{\beta_0} = 0. \tag{B.2}$$

This gives

$$E = -\left(\frac{\partial}{\partial \beta}\ln Z_N\right)_{\beta_0}. \tag{B.3}$$

This is in fact the thermodynamic definition of the ensemble average E for an equilibrium temperature $1/\beta_0$. Next, expanding $S_N(\beta)$ about the stationary point β_0,

$$S_N(\beta) = S_N(\beta_0) + \frac{1}{2!}(\beta - \beta_0)^2 S_N''(\beta_0) + \ldots.$$

Substituting this in the expression for $\rho_N(E)$, we obtain the smooth part of the density of states $\bar{\rho}_N(E)$:

$$\bar{\rho}_N(E) = \frac{e^{S(\beta_0)}}{2\pi i}\int_{-i\infty}^{i\infty} exp\left[(\beta - \beta_0)^2 S_N''(\beta_0)/2\right].$$

Letting $\beta - \beta_0 = ix$, the integral becomes [111]:

$$\begin{aligned} \bar{\rho}_N(E) &= \frac{e^{S_N(\beta_0)}}{2\pi} \int_{-\infty}^{\infty} e^{-S_N''(\beta_0)\ x^2/2}, \\ &= \frac{e^{S_N(\beta_0)}}{\sqrt{2\pi S_N''(\beta_0)}} \ . \end{aligned} \tag{B.4}$$

Appendix C

Addendum to section 4.1.2

The followings are two Maple programs for calculating the microstate and the number fluctuation for ideal fermions in an one-dimensional harmonic trap. The first determines the multiplicity using direct combinatorial counting (function Part()), while the second uses the method outlined in section 4.1.2.

Version 1.

Initialization.

```
> restart; N:=3:  nmax:=10:
```

Function Part() partitions an integer n into at most M parts, whose part value <=NH, the number of level defined for hole states. For particle spaces put NH >=n.

```
> Part:=proc(n,NH,M,t)
local i:  global count:
if NH=0 or NH=1 then
if t+n<=M then count:=count+1 else count:=count fi:  else
for i from 1 to NH do Part(n-i,min(n-i,i),M,t+1) od:
fi:  count; end:
```

Coefficients Omegah( ) for the hole space.

```
> for n from 0 to nmax do
for Nex from 1 to N do Omegah(n,Nex):=0 od:  od:
if type(N,odd)=true then Nmid:=(N-1)/2 else Nmid:=N/2 fi:
for Nex from 2 to Nmid do:
NH:=N-Nex; numterm:=NH*Nex;
for n from 2 to numterm do:
count:=0:
```

```
Omegah(n,Nex):=Part(n,NH,Nex,0):  Omegah(n,NH):=Omegah(n,Nex):
#print(n,Nex,Omegah(n,Nex));
od:
Omegah(0,Nex):=1:Omegah(1,Nex):=1:  Omegah(0,NH):=1:Omegah(1,NH):=1:
od:
for n from 0 to N-1 do:  Omegah(n,1):=1:  Omegah(n,N-1):=1:  od:
```

Partition function of an one-dimensional harmonic trap, expanded in power of x. Call this Zp-partition function for particle space.

```
>  S(0):=0:
for Nx from 1 to N do:
Zp(Nx):=product(1/(1-x^j),j=1..Nx):
Sp(Nx):=series(Zp(Nx),x=0,nmax+1):
od:
```

Calculate the microstates and and the ground state number fluctuation as function of E=n.

```
>  fluc(0):=0:fluc(1):=0:
barnot(0):=N:barnot(1):=N-1:
for n from 2 to nmax do:
for Nex from 1 to N do:
nhmin:=(Nex-1)*Nex/2:  npmin:=(Nex+1)*Nex/2:  nhmax:=n-npmin:
if nhmax > nhmin then
ncutoff:=nhmax-nhmin:
w(n,Nex):=add(Omegah(a,Nex)*coeff(Sp(Nex),x^(ncutoff-a)),a=1..ncutoff- 1)+
coeff(Sp(Nex),x^ncutoff)+Omegah(ncutoff,Nex):
elif nhmax=nhmin then w(n,Nex):=1:  else w(n,Nex):=0:  fi:
#if w(n,Nex) > 0 then print(n,Nex,w(n,Nex)) fi;
P(n,Nex):=w(n,Nex)/coeff(Sp(N),x^n):
od:
bar(n):= sum(L*P(n,L),L=1..N): barnot(n):=evalf(N-bar(n)):
sqbar(n):=sum(J^2*P(n,J),J=1..N): fluc(n):=evalf(sqrt(sqbar(n)-bar(n)^2)/N):
od:
```

Results.

```
>  print(w(5,1),w(5,2),w(5,3));
```

$$3, 2, 0.$$

Version 2.

Initialization.

```
> restart; with(linalg):  N:=3:  nmax:=10:
```

Define matrices to store the Omega_p, Omega_h.

```
> A:=array(sparse,1..N,1..nmax+1):  B:=array(sparse,1..N,1..nmax+1):
for m from 1 to N do A[m,1]:=1:  B[m,1]:=1:  od:
```

Procedure for the recursive formula (Eq. 4.8).

```
> parth:=proc(M)
local j:
if M=0 then 1 elif M=1 then Z1(1) else
for j from 1 to M do:  temp(j,M):=simplify(Z1(j)*parth(M-j)):od:
sum(temp(i,M),i=1..M)/M:fi:
end:
```

Partition functions for the hole space.

```
> Zh(N):=1:
if type(N,odd)=true then Nmid:=(N-1)/2 else Nmid:=N/2 fi:
for nex from 1 to Nmid do:
NH:=N-nex:
Z1:=j->sum(x^(j*n),n=0..NH): Zh(nex):=parth(nex):  Zh(NH):=Zh(nex):
od:
for ii from 1 to N do:  Sh(ii):=series(Zh(ii),x=0,degree(Zh(ii))+1):  od:
```

Partition functions for the particle space.

```
> S(0):=0:
for Nx from 1 to N do:
Zp(Nx):=product(1/(1-x^j),j=1..Nx):  Sp(Nx):=series(Zp(Nx),x=0,nmax+1):
od:
```

Extracting the macrostates.

```
> for i from 1 to N do
for j from 2 to degree(Zh(i))+1 do A[i,j]:=coeff(Sh(i),x^(j-1)):  od:
for k from 2 to nmax+1 do B[i,k]:=coeff(Sp(i),x^(k-1)):  od:
od::
```

Print to files.

```
> file1:=fopen(`fOmegah10.mat`,WRITE):
file2:=fopen(`fOmegap10.mat`, WRITE):
> writedata(file1,A,integer);writedata(file2,B,integer);
```

```
> fclose(file1):fclose(file2):
```

Using the stored values of the multiplicities, the fluctuation may then easily be calculated using any computer programming language. As a representation, we next list the partition functions for both particle and hole spaces for $N = 10$.

Particle Space.

$$
\begin{aligned}
Z_1 &= 1 + x + x^2 + x^3 + x^4 + x^5 + x^6 + x^7 + x^8 + x^9 + x^{10} + x^{11} + x^{12} + x^{13} + \ldots, \\
Z_2 &= 1 + x + 2\,x^2 + 2\,x^3 + 3\,x^4 + 3\,x^5 + 4\,x^6 + 4\,x^7 + 5\,x^8 + 5\,x^9 + 6\,x^{10} + \\
&\quad 6\,x^{11} + 7\,x^{12} + 7\,x^{13} + 8x^{14} + 8\,x^{15} + \ldots, \\
Z_3 &= 1 + x + 2\,x^2 + 3\,x^3 + 4\,x^4 + 5\,x^5 + 7\,x^6 + 8\,x^7 + 10\,x^8 + 12\,x^9 + 14\,x^{10} + \\
&\quad 16\,x^{11} + 19\,x^{12} + 21x^{13} + 24\,x^{14} + 27\,x^{15} + \ldots, \\
Z_4 &= 1 + x + 2\,x^2 + 3\,x^3 + 5\,x^4 + 6\,x^5 + 9\,x^6 + 11\,x^7 + 15\,x^8 + 18\,x^9 + 23\,x^{10} + \\
&\quad 27\,x^{11} + 34\,x^{12} + 39\,x^{13} + 47\,x^{14} + 54\,x^{15} + \ldots, \\
Z_5 &= 1 + x + 2\,x^2 + 3\,x^3 + 5\,x^4 + 7\,x^5 + 10\,x^6 + 13\,x^7 + 18\,x^8 + 23\,x^9 + 30\,x^{10} + \\
&\quad 37\,x^{11} + 47\,x^{12} + 57\,x^{13} + 70\,x^{14} + 84\,x^{15} + \ldots, \\
Z_6 &= 1 + x + 2\,x^2 + 3\,x^3 + 5\,x^4 + 7\,x^5 + 11\,x^6 + 14\,x^7 + 20\,x^8 + 26\,x^9 + 35\,x^{10} + \\
&\quad 44\,x^{11} + 58\,x^{12} + 71\,x^{13} + 90\,x^{14} + 110\,x^{15} + \ldots, \\
Z_7 &= 1 + x + 2\,x^2 + 3\,x^3 + 5\,x^4 + 7\,x^5 + 11\,x^6 + 15\,x^7 + 21\,x^8 + 28\,x^9 + 38\,x^{10} + \\
&\quad 49\,x^{11} + 65\,x^{12} + 82\,x^{13} + 105\,x^{14} + 131\,x^{15} + \ldots, \\
Z_8 &= 1 + x + 2\,x^2 + 3\,x^3 + 5\,x^4 + 7\,x^5 + 11\,x^6 + 15\,x^7 + 22\,x^8 + 29\,x^9 + 40\,x^{10} + \\
&\quad 52\,x^{11} + 70\,x^{12} + 89\,x^{13} + 116\,x^{14} + 146\,x^{15} + \ldots, \\
Z_9 &= 1 + x + 2\,x^2 + 3\,x^3 + 5\,x^4 + 7\,x^5 + 11\,x^6 + 15\,x^7 + 22\,x^8 + 30\,x^9 + 41\,x^{10} + \\
&\quad 54\,x^{11} + 73\,x^{12} + 94\,x^{13} + 123\,x^{14} + 157\,x^{15} + \ldots, \\
Z_{10} &= 1 + x + 2\,x^2 + 3\,x^3 + 5\,x^4 + 7\,x^5 + 11\,x^6 + 15\,x^7 + 22\,x^8 + 30\,x^9 + 42\,x^{10} + \\
&\quad 55\,x^{11} + 75\,x^{12} + 97\,x^{13} + 128\,x^{14} + 164\,x^{15} + \ldots.
\end{aligned}
$$

Hole Space.

$$
\begin{aligned}
Z_1^h &= 1+x+x^2+x^3+x^4+x^5+x^6+x^7+x^8+x^9,\\
Z_2^h &= 1+x+2\,x^2+2\,x^3+3\,x^4+3\,x^5+4\,x^6+4\,x^7+5\,x^8+4\,x^9+4\,x^{10}+\\
&\quad 3\,x^{11}+3\,x^{12}+2\,x^{13}+2x^{14}+x^{15}+x^{16},\\
Z_3^h &= 1+x+2\,x^2+3\,x^3+4\,x^4+5\,x^5+7\,x^6+8\,x^7+9\,x^8+10\,x^9+10\,x^{10}+\\
&\quad 10\,x^{11}+10\,x^{12}+9x^{13}+8\,x^{14}+7\,x^{15}+5\,x^{16}+4\,x^{17}+3\,x^{18}+2\,x^{19}+x^{20}+x^{21},\\
Z_4^h &= 1+x+2\,x^2+3\,x^3+5\,x^4+6\,x^5+9\,x^6+10\,x^7+13\,x^8+14\,x^9+16\,x^{10}+\\
&\quad 16\,x^{11}+18\,x^{12}+16\,x^{13}+16\,x^{14}+14\,x^{15}+13\,x^{16}+10\,x^{17}+9\,x^{18}+6\,x^{19}+\\
&\quad 5\,x^{20}+3\,x^{21}+2\,x^{22}+x^{23}+x^{24},\\
Z_5^h &= 1+x+2\,x^2+3\,x^3+5\,x^4+7\,x^5+9\,x^6+11\,x^7+14\,x^8+16\,x^9+18\,x^{10}+\\
&\quad 19\,x^{11}+20\,x^{12}+20\,x^{13}+19\,x^{14}+18\,x^{15}+16\,x^{16}+14\,x^{17}+11\,x^{18}+9\,x^{19}+\\
&\quad 7\,x^{20}+5\,x^{21}+3\,x^{22}+2x^{23}+x^{24}+x^{25},\\
Z_6^h &= 1+x+2\,x^2+3\,x^3+5\,x^4+6\,x^5+9\,x^6+10\,x^7+13\,x^8+14\,x^9+16\,x^{10}+\\
&\quad 16\,x^{11}+18\,x^{12}+16\,x^{13}+16\,x^{14}+14\,x^{15}+13\,x^{16}+10\,x^{17}+9\,x^{18}+6\,x^{19}+\\
&\quad 5\,x^{20}+3\,x^{21}+2\,x^{22}+x^{23}+x^{24},\\
Z_7^h &= 1+x+2\,x^2+3\,x^3+4\,x^4+5\,x^5+7\,x^6+8\,x^7+9\,x^8+10\,x^9+10\,x^{10}+\\
&\quad 10\,x^{11}+10\,x^{12}+9x^{13}+8\,x^{14}+7\,x^{15}+5\,x^{16}+4\,x^{17}+3\,x^{18}+2\,x^{19}+x^{20}+x^{21},\\
Z_8^h &= 1+x+2\,x^2+2\,x^3+3\,x^4+3\,x^5+4\,x^6+4\,x^7+5\,x^8+4\,x^9+4\,x^{10}+\\
&\quad 3\,x^{11}+3\,x^{12}+2\,x^{13}+2x^{14}+x^{15}+x^{16},\\
Z_9^h &= 1+x+x^2+x^3+x^4+x^5+x^6+x^7+x^8+x^9,\\
Z_{10}^h &= 1.
\end{aligned}
$$

As expected, the partition functions for the hole space are finite.

Appendix D

Calculation of T_C of N ideal bosons in a one-dimensional harmonic trap

The population of a state with energy ϵ_i is given by the usual Bose-Einstein distribution

$$\langle n_i \rangle = \frac{1}{e^{(\epsilon_i - \mu)\beta} - 1} = \frac{ze^{-\epsilon_i \beta}}{1 - ze^{-\epsilon_i \beta}}, \tag{D.1}$$

where $z = e^{\mu\beta}$ is the fugacity. The energy of the ground state has been taken to be zero. The ground state occupancy is $N_0 = z/(1-z)$. The total number of particles is determined from

$$\begin{aligned} N &= \sum_{i=0}^{\infty} \langle n_i \rangle = \sum_{i=0}^{\infty} \frac{ze^{-\epsilon_i\beta}}{1 - ze^{-\epsilon_i\beta}} = \sum_{i=0}^{\infty} ze^{-\epsilon_i\beta} \sum_{j=0}^{\infty} z^j e^{-j\epsilon_i\beta}, \\ &= \sum_{i=0}^{\infty} \sum_{j=1}^{\infty} z^j e^{-j\epsilon_i\beta}. \end{aligned} \tag{D.2}$$

The above result is general for any single-particle spectrum $\{\epsilon_i\}$. We now apply it to a one-dimensional harmonic trap. The spectrum is given by $\epsilon_i = i\hbar\omega,\ i = 0, 1, 2, \ldots$. Eq. (D.2) becomes

$$\begin{aligned} N &= \sum_{i=0}^{\infty} \sum_{j=1}^{\infty} z^j e^{-ij\hbar\omega\beta}, \\ &= \sum_{j=1}^{\infty} z^j \sum_{i=0}^{\infty} e^{-ij\hbar\omega\beta}. \end{aligned}$$

The second summation is a geometric progression series. This may be summed to give

$$\begin{aligned} N &= \sum_{j=1}^{\infty} z^j \frac{1}{1-e^{-j\hbar\omega\beta}}, \\ &= \frac{z}{1-z} + \sum_{j=1}^{\infty} \frac{z^j e^{-j\hbar\omega\beta}}{1-e^{-j\hbar\omega\beta}}. \end{aligned}$$

For $\hbar\omega\beta \ll 1$ (the temperature is larger than the level spacing), the above is approximated by

$$N = N_0 + \frac{1}{\hbar\omega\beta} \sum_{j=1}^{\infty} \frac{\left[ze^{-\hbar\omega\beta/2}\right]^j}{j} = N_0 - \frac{1}{\hbar\omega\beta} \ln\left[1 - ze^{-\hbar\omega\beta/2}\right]. \tag{D.3}$$

The transition temperature is found by letting $z \to 1$ and $N_0 \to 0$. Thus

$$N = \frac{T_c}{\hbar\omega} \ln\left(\frac{2T_c}{\hbar\omega}\right) \tag{D.4}$$

To solve for T_c, we replace $T_c = \hbar\omega N$ in the logarithmic in the first approximation:

$$T_c = \frac{\hbar\omega N}{\ln\left(\frac{2T_c}{\hbar\omega}\right)} \approx \hbar\omega \frac{N}{\ln(2N)}. \tag{D.5}$$

The transition temperature may also be obtained from the density of state approach. From Eq. (4.27), with $\rho(\epsilon) = 1/\hbar\omega$,

$$N - N_0 = \int \rho(\epsilon) \frac{ze^{-\epsilon_i\beta}}{1-ze^{-\epsilon_i\beta}} d\epsilon = \frac{1}{\hbar\omega} \sum_{j=1}^{\infty} z^j \int e^{-j\epsilon\beta} d\epsilon. \tag{D.6}$$

To avoid low frequency divergence, the lower limit in the integral is set to be $\hbar\omega/2$. Thus,

$$\begin{aligned} N - N_0 &= \frac{1}{\hbar\omega} \sum_{j=1}^{\infty} z^j \int_{\hbar\omega/2}^{\infty} e^{-j\epsilon\beta} d\epsilon, \\ &= \frac{1}{\hbar\omega\beta} \sum_{j=1}^{\infty} \frac{z^j e^{-j\hbar\omega\beta/2}}{j}, \end{aligned}$$

which is the same as Eq. (D.3).

Appendix E

List of $\Omega(E)$ for the $\ln n$ spectrum

Tabulation of the many-body multiplicity $\Omega(E_n)$, with $N \to \infty$. The many-body eigenenergy spectrum $E_n = \ln n$. The single-particle is $\epsilon_n = \ln n$ and is nondegenerate.

n	E_n	$\Omega(E_n)$	n	E_n	$\Omega(E_n)$	n	E_n	$\Omega(E_n)$
1	0	1	34	3.526360525	2	67	4.204692619	1
2	.6931471806	1	35	3.555348061	2	68	4.219507705	4
3	1.098612289	1	36	3.583518938	9	69	4.234106505	2
4	1.386294361	2	37	3.610917913	1	70	4.248495242	5
5	1.609437912	1	38	3.637586160	2	71	4.262679877	1
6	1.791759469	2	39	3.663561646	2	72	4.276666119	14
7	1.945910149	1	40	3.688879454	7	73	4.290459441	1
8	2.079441542	3	41	3.713572067	1	74	4.304065093	2
9	2.197224577	2	42	3.737669618	5	75	4.317488114	4
10	2.302585093	2	43	3.761200116	1	76	4.330733340	4
11	2.397895273	1	44	3.784189634	4	77	4.343805422	2
12	2.484906650	4	45	3.806662490	4	78	4.356708827	5
13	2.564949357	1	46	3.828641396	2	79	4.369447852	1
14	2.639057330	2	47	3.850147602	1	80	4.382026635	12
15	2.708050201	2	48	3.871201011	12	81	4.394449155	5
16	2.772588722	5	49	3.891820298	2	82	4.406719247	2
17	2.833213344	1	50	3.912023005	4	83	4.418840608	1
18	2.890371758	4	51	3.931825633	2	84	4.430816799	8
19	2.944438979	1	52	3.951243719	4	85	4.442651256	2
20	2.995732274	4	53	3.970291914	1	86	4.454347296	2
21	3.044522438	2	54	3.988984047	7	87	4.465908119	2
22	3.091042453	2	55	4.007333185	2	88	4.477336814	7
23	3.135494216	1	56	4.025351691	7	89	4.488636370	1
24	3.178053830	7	57	4.043051268	2	90	4.499809670	11
25	3.218875825	2	58	4.060443011	2	91	4.510859507	2
26	3.258096538	2	59	4.077537444	1	92	4.521788577	4
27	3.295836866	3	60	4.094344562	10	93	4.532599493	2
28	3.332204510	4	61	4.110873864	1	94	4.543294782	2
29	3.367295830	1	62	4.127134385	2	95	4.553876892	2
30	3.401197382	5	63	4.143134726	4	96	4.564348191	19
31	3.433987204	1	64	4.158883083	11	97	4.574710979	1
32	3.465735903	7	65	4.174387270	2	98	4.584967479	4
33	3.496507561	2	66	4.189654742	5	99	4.595119850	4

Appendix F

Addendum to section 5.2.3

We consider N particles, either bosons or fermions, interacting in the CSM whose Hamiltonian is given by Eq. (5.8). In the thermodynamic limit, which is obtained by taking $\omega \to 0$ as $N \to \infty$ such that $\omega N =$ constant, the correlation functions are known exactly for three values of g [76]:

$$g = 1: \quad \nu(r) = s(r)^2 = \left[\frac{\sin(\pi r)}{\pi r}\right]^2 \tag{F.1}$$

$$g = 1/2: \nu(r) = s(r)^2 + \frac{ds}{dr}\int_r^{\infty} dt\ [s(t)] \tag{F.2}$$

$$g = 2: \quad \nu(r) = s(2r)^2 - \frac{ds(2r)}{dr}\int_0^{2r} dt\ [s(t)], \tag{F.3}$$

where the Fermi momentum k_F is set equal to π so that the maximum central density is unity. Let $\nu(r)$ denotes the two-particle ground state density-density correlation function in the ground state, with $r = |x_1 - x_2|$, then the number fluctuation is related to the correlation function as [1]

$$\frac{(\delta N)^2}{N} - 1 = -\int_{-\infty}^{\infty} \nu(r)dr. \tag{F.4}$$

Note that the ground state correlation function $\nu(r)$ is defined only for $r \geq 0$. However, in computing the above integral it is necessary to assume $\nu(r)$ to be even function, and extend the domain of integration to negative values of r [112].

g=1:

$$-2\int_0^{\infty} \nu(r)dr = -2\int_0^{\infty}\left[\frac{\sin(\pi r)}{\pi r}\right]^2 = -1. \tag{F.5}$$

g=1/2:

$$-2\int_0^{\infty} \nu(r)dr = -2\int_0^{\infty} s(r)^2 dr - 2\int_0^{\infty}\left[\int_r^{\infty} s(t)dt\right] s'(r)dr = -1. \tag{F.6}$$

g=2:

$$-2\int_0^\infty \nu(r)dr = -2\int_0^\infty s(2r)^2 dr + 2\int_0^\infty \left[\int_0^{2r} s(t)dt\right] s'(2r)dr = -1. \tag{F.7}$$

Thus it follows that for interacting bosons in CSM the fluctuation vanishes identically at $T = 0$.

While we cannot obtain the exact $\nu(r)$ in CSM for all g, the same may be calculated for all values of g in the harmonic lattice approximation. The correlation function so obtained compares very well with the exact correlation functions for $g = 1/2, 1, 2$ and is given by [113]

$$\nu(x) = \rho_0 \sum_{i\neq 0} \left(\frac{1}{4\pi F(i,0)}\right)^{1/2} \exp\left[-\frac{(x\rho_0 - i)^2}{4F(i,0)}\right] - \rho_0, \tag{F.8}$$

where $\rho_0 = N/L$ is the average density and

$$gF(i,0) = \frac{1}{2\pi^2}\int_0^\pi dy \frac{1-\cos(yi)}{y - y^2/2\pi} = \frac{1}{2\pi^2}\int_0^{2\pi} dy\ \frac{1-\cos(yi)}{y}. \tag{F.9}$$

The above expression is given for completeness and its exact form is not needed for further calculations. Again integrating over the real line we get a result identical to that obtained using the exact correlation functions in CSM. Thus the fluctuation vanishes identically for all g in this approximation at zero temperature.

Appendix G

Ultra Low temperature expansions in the GCE and CE

The low temperature behaviour of thermodynamic quantities in the GCE are well known for bosonic systems. However, a comparison between the grand canonical and the canonical calculations at low temperatures is not usually discussed for either Bose or Fermi systems. Further, making use of some asymptotic expansions, the canonical number fluctuation for bosons in a one-dimensional harmonic trap was earlier found to be linear right down to $T = 0$ [9, 26]. However, we give here the expansion of the fluctuation squared at low temperature in power of x, where $x = e^{-\beta\omega}$, and show that the canonical fluctuation of bosons is in fact exponential at very low T. In the GCE only expansion for fermions is possible, since the fluctuation tends to infinity at low temperature for bosons. Both expansions are possible in the CE.

Grand Canonical Ensemble In the GCE the (fermionic) occupation number is:

$$\langle n_k \rangle_{GCE} = \frac{1}{x^{(\mu-\epsilon_k)}+1} = \frac{1}{x^{(\mu-k-1/2)}+1} \tag{G.1}$$

for a one-dimensional harmonic trap. The ground state number fluctuation squared is given by:

$$\langle \triangle N_0^2 \rangle_{GCE} = \sum_{k=0}^{k_F} \frac{x^{(\mu-k-1/2)}}{\left[x^{(\mu-k-1/2)}+1\right]^2} \tag{G.2}$$

where k_F is the Fermi level. At low temperatures, for the one-dimensional harmonic oscillator, $\mu \approx \mu_0 = N$. Therefore,

$$\begin{aligned}
\langle \triangle N_0^2 \rangle_{GCE} &= \sqrt{x} - 2x + 3x^{3/2} - 4x^2 + 5x^{5/2} - 6x^3 + 7x^{7/2} - 8x^4 + \ldots, \quad N = 1. \\
&= \sqrt{x} - 2x + 4x^{3/2} - 4x^2 + 5x^{5/2} - 8x^3 + 7x^{7/2} - 8x^4 + \ldots, \quad N = 2. \\
&= \sqrt{x} - 2x + 4x^{3/2} - 4x^2 + 6x^{5/2} - 8x^3 + 7x^{7/2} - 8x^4 + \ldots, \quad N = 1. \\
&= \sqrt{x} - 2x + 4x^{3/2} - 4x^2 + 6x^{5/2} - 8x^3 + 8x^{7/2} - 8x^4 + \ldots, \quad N = 4.
\end{aligned}$$

Thus,

$$\langle \triangle N_0^2 \rangle_{GCE} = \sqrt{x} - 2x + 4x^{3/2} - 4x^2 + 6x^{5/2} - 8x^3 + 8x^{7/2} - 8x^4 + \ldots, \quad N \geq 4. \tag{G.3}$$

Note that the terms up to $O(x^4)$ are independent of N for $N \geq 4$.

Canonical Ensemble In the CE the first and second moments of the occupation number are given by Eqs. (2.18) and (2.19):

$$\langle n_k \rangle = \frac{1}{Z_N} \sum_j^N (\pm)^{j+1} x^{j\epsilon_k} Z_{N-j}, \tag{G.4}$$

$$\langle n_k^2 \rangle = \frac{1}{Z_N} \sum_j^N (\pm)^{j+1} \left[j \pm (j-1) \right] x^{j\epsilon_k} Z_{N-j}, \tag{G.5}$$

where the upper and lower signs refer to bosons and fermions respectively. Summing over the ground states up the Fermi level gives the fermionic ground state number:

$$\langle N_0 \rangle_{CE} = \frac{1}{Z_N} \sum_j^N (-1)^{j+1} x^{j/2} \frac{1 - x^{jN}}{1 - x^j} Z_{N-j}, \tag{G.6}$$

where we let $\epsilon_k = k - 1/2$, with $k = 1, 2, \ldots$. Therefore,

$$\begin{aligned}
\langle \Delta N_0^2 \rangle_{CE} &= \sum_{k=1}^N \langle n_k \rangle - \sum_{k=1}^N \langle n_k \rangle^2 \\
&= x + 2x^4 + \ldots \quad , \quad N \geq 4,
\end{aligned} \tag{G.7}$$

where we have used $\langle n_k \rangle = \langle n_k^2 \rangle$ and again the first few terms are independent of the system size N for $N \geq 4$.

For bosons the ground state consists of one single lowest level, the low temperature expansion of the number fluctuation is given by

$$\begin{aligned} \langle \triangle N_0^2 \rangle \rangle_{CE} &= \langle n_0^2 \rangle - \langle n_0 \rangle^2 \\ &= x + 3x^2 + 4x^3 + 7x^4 + \ldots \quad , \quad N > 4. \end{aligned} \tag{G.8}$$

Again as in the fermionic case the first few terms in the low temperature expansions are independent of the system size. Indeed it is interesting to note that in CE, the fluctuations in both systems approach zero as $T \to 0$ in exactly identical fashion.

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