Chapter 3

Statistical fluctuation and thermodynamic properties

3.1 Statistical fluctuation in ideal Bose gas

Study of statistical fluctuation and thermodynamic properties of bosonic systems are old textbook problems [85, 91, 92, 93, 94]. Ideal Bose gas in one, two and three dimension have been studied in great detail [95, 96, 97, 98, 99, 100]. At earlier times it was predicted that phase transition (transition from normal Bose gas to condensation) is not possible in lower dimensions [97, 101, 102, 103, 104, 105]. But Druten *et al.* had shown that phase transition is possible in 1D [106]. Static and thermodynamic properties of weakly interacting bosonic system were studied by several groups [102, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117]. Earlier calculations of average properties such as the condensate fraction, critical temperature and atom number fluctuation of the ground state were mainly performed considering grand canonical ensemble (GCE) approach [95, 96, 101, 102, 112, 115, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127]. In GCE the system is connected with a reservoir, so the exchange of both energy and particle number are allowed. Fluctuation in the occupation number for i-th energy state can be written as $\delta N_i^2 = N_i(N_i - 1)$. Above the transition temperature, it predicts the correct result for the fluctuation in the ground state occupation number where one can imagine the excited states as the reservoir for the ground state atoms. Below or around the critical temperature, most of the particles occupy the ground state.

Then the fluctuation in the ground state must die out but GCE ensemble predicts that the fluctuation is of the order of the size of the system i.e., $\delta N_0 \propto N_0$ - this is called the grand canonical catastrophe [117, 125, 126, 127, 128, 129, 130]. This GCE representation for ideal Bose gas had already been pointed out by several groups [131, 132, 133, 134]. The constraints considered in GCE i.e., both energy and particle number can be exchanged is in sharp contrast with the experimental arrangement where the atoms are trapped so total number of particles are fixed. Due to this constraint of particle number exchange, the result obtained by GCE approach is questionable. To explain the experimental observation and predict correct new physics, one needs to consider the microcanonical or canonical ensemble approach.

3.2 Statistical fluctuation in interacting Bose gas

The preceding discussion was mainly focused to describe the study of fluctuation properties for the non-interacting or ideal Bose gas. However, in experiments, people deal with the interacting Bose gas in harmonic oscillator trap. It is experimentally observed that, due to the inhomogeneity, even the weak-interaction has significant effect on the measures of several thermodynamic properties. As the inclusion of the interaction makes the many-body problem nontrivial, most theoretical results in this direction are mainly centered on the homogeneous case. Due to the GCE catastrophe, several methodologies emerge which consider a canonical or microcanonical approach to properly address fluctuations in interacting Bose gas. Giorgini et al. calculated fluctuation in interacting Bose gas by Bogoliubov quasi-particle approach [135]. They have reproduced the non-interacting limiting case as found in the work of Politzer et al. [118]. Later, Kocharovsky et al. published a series of works to extend the idea of this methodology [107, 109, 136, 137]. They have also used another methodology which is based on the number conserving canonical approach [108, 138] and studied condensate fraction and several orders of central moment. A hybrid master equation approach was also introduced to calculate several properties of BEC [139, 140] which gives anomalous fluctuation. But Idziaszek et al. [141] had shown that the fluctuation is linearly proportional to the particle number. Fluctuation in interacting Bose gas has been calculated by several other groups by exact recursion relation method [112, 115, 111, 110, 142, 143]. However, none of the above methodologies deal with the experimental situation of JILA and RICE trap. The first attempt had been taken by Chakrabarti and Bhattacharyya [43] to study the fluctuation of repulsive BEC in JILA trap. Experimental observation of statistical fluctuation for repulsively interacting BEC in harmonic oscillator can be found in the Ref. [144]. However, the effect of attractive interaction and anisotropy in the trap are still an unsolved area of research. So, we will discuss the effect of interaction and trapping potential on several statistical properties like condensate fraction, fluctuation in the ground state occupation number, several orders of central moment and specific heat. All these properties have been measured very minutely for the whole temperature region to describe the process of phase transition from condensation to normal Bose gas.

3.3 Recursion relation to calculate partition function

For the present study, we start from the canonical ensemble which takes care of the intermediate situation of the microcanonical ensemble and the grand canonical ensemble - so is the most appealing one. In the microcanonical ensemble, the gas is completely isolated and there is no exchange of energy or atoms so it gives some over-estimated values for several statistical properties. Whereas in the grand-canonical ensemble, only the average energy per atom and the average number of atoms are fixed, thus there is an exchange of both energy and atoms which leads to the grand canonical catastrophe [117, 125, 126, 127, 128, 129, 130].

P. T. Landsberg first proposed a recursion method [131] to calculate the partition function for the canonical ensemble with moderate atom numbers and an iteration procedure with respect to the number of particles was used. Later, Landsberg's method was improved by E. D. Trifonov *et al.* [142] to facilitate its application for a larger number of particles and a wider temperature range. It also demonstrates the efficiency of recursion technique for three dimensional isotropic trapped ideal Bose gas. For completeness, here we briefly summarize the method which we utilize in our numerical calculation.

The probability of the N-particle system in a state, described by an occupation number $\{n_i\}$, is given by

$$P_{\{n_i\}} = \frac{1}{Z_N} \exp\left(-\frac{E_{\{n_i\}}}{k_B T}\right),$$
(3.1)

where Z_N is the partition function of the N-particle system and can be defined as,

$$Z_N = \sum_{\{n_i\}} \exp\left(-\frac{E_{\{n_i\}}}{k_B T}\right) \tag{3.2}$$

with the summation performed over all combinations of the occupation numbers that satisfy the condition

$$\sum_{i} n_i = N. \tag{3.3}$$

Thus the probability of finding n_k particles in k-th single particle state is determined as

$$P_{n_k}^{(k)} = \frac{Z_{N-n_k}^{(k)}}{Z_N} \exp\left(-\frac{n_k E_k}{k_B T}\right).$$
 (3.4)

where $Z_{N-n_k}^{(k)}$ is the partition function for $(N - n_k)$ particles, with the k-th single particle state excluded from the sum. E_k is the energy of the k-th single particle state.

In terms of Landsberg's recursion method, using iteration with respect to the number of particles, the partition function can be calculated by a simple algorithm [142] as

$$Z_n = \frac{1}{n} \sum_{p=1}^n S_p Z_{n-p}, \ Z_0 = 1; \ n = 1, 2, ..., N$$
(3.5)

where,

$$S_p = \sum_j \exp(-\frac{pE_j}{k_B T}). \tag{3.6}$$

This is an ideal method where, the summation can be performed analytically like three dimensional isotropic harmonic trap. Landsberg's method was used to calculate the partition function of Bose gas with moderate particle number (~ 100) and for sufficiently low temperature $T \ll T_c$ [131]. For our many particle system, the energy of a state (n, l) is E_{nl} . The the above equation takes the form

$$S_p = \sum_{n=0}^{n_{max}} \sum_{l=0}^{l_{max}} (2l+1) \exp(-\frac{pE_{nl}}{k_B T}).$$
(3.7)

The limits for n_{max} and l_{max} are described in the methodology section. Later, Trifonov *et al.* improved Landsberg's methodology for larger particle number and increasing temperature [142]. The recursion formulas are:

$$Z_0^{\{0\}} = 1 \quad , \tag{3.8}$$

$$Z_n^{\{n-1\}} = \sum_{p=0}^{n-1} \frac{S_{n-p} Z_p^{\{n-1\}}}{n}, \ n = 1, \dots, N,$$
(3.9)

$$Z_k^{\{n\}} = \frac{Z_k^{\{n-1\}}}{\sum_{p=0}^n Z_p^{\{n-1\}}}, \quad k = 0, \dots, n.$$
(3.10)

The probability of finding n_0 particles out of total particle N in the ground state is

$$P_{n_0} = Z_{N-n_0}^{\{N\}},\tag{3.11}$$

where

$$Z_N = Z_N^{\{N\}} \prod_{n=1}^N \sum_{p=0}^n Z_p^{\{n-1\}}.$$
(3.12)

The relation between the probability distribution of n_0 number of atoms in the ground states P_{n_0} and the canonical partition function is given by

$$P_{n_0} = \frac{Z_{N-n_0}(T) - Z_{N-n_0-1}(T)}{Z_N(T)}$$
(3.13)

Accordingly the mean number of particles in the ground state and its rootmean-square fluctuation can be found from the relation

$$\langle n_0 \rangle = \sum_{n_0=0}^{N} n_0 P_{n_0}$$
 (3.14)

and

$$\delta n_0 = \sqrt{\langle n_0^2 \rangle - \langle n_0 \rangle^2} \tag{3.15}$$

where

$$< n_0^2 > = \sum_{n_0=0}^N n_0^2 P_{n_0}.$$
 (3.16)

Central moments are obtained as

$$<\left(n_{0}-< n_{0}>\right)^{m}> = \sum_{n_{0}=0}^{N}\left(n_{0}-< n_{0}>\right)^{m}P_{n_{0}}.$$
 (3.17)

The moment with m = 2 is defined as the standard deviation and m = 3, 4 are defined as the third- and fourth-order central moments respectively.

3.3.1 Calculation of specific heat

For a fixed temperature T, the distribution of N number of bosons in the energy level E_{nl} according to the Bose distribution can be written as

$$f(E_{nl}) = \frac{1}{e^{\beta(E_{nl}-\mu)} - 1}$$
(3.18)

The average energy E(N,T) of the system at any temperature T can be obtained as

$$E(N,T) = \sum_{n=0}^{\infty} \sum_{l=0}^{\infty} (2l+1)f(E_{nl})E_{nl}.$$
(3.19)

The heat capacity $C_N(T)$ at a fixed N is calculated by the partial derivative of E(N,T) with respect to T as

$$C_N(T) = \beta \sum_{n=0}^{\infty} \sum_{l=0}^{\infty} \frac{(2l+1)E_{nl}e^{\beta(E_{nl}-\mu)}}{(e^{\beta(E_{nl}-\mu)}-1)^2} \Big[\frac{(E_{nl}-\mu)}{T} + \frac{\partial\mu}{\partial T}\Big],$$
(3.20)

where chemical potential μ is a function of T, $\beta = \frac{1}{k_B T}$, where k_B is the Boltzmann's constant.