## Chapter 6

# Effect of interaction on energy fluctuation of BEC in harmonic trap

Several thermodynamic properties and condensate fluctuations for ideal Bose gas (IBG) as well as weakly interacting Bose gas are reported in several important earlier works [43, 94, 107, 108, 113, 115, 123, 125, 140, 146]. However, the calculation of energy fluctuation of N interacting atoms trapped in harmonic confinement is not rigorously studied yet. Two-body interaction and correlation between the atoms play an crucial role in the attractive interacting BEC. Since, a collapse is always related with the attractive interacting trapped Bose gas so, in such mesoscopic systems, the study of energy fluctuation is very challenging. Though, the energy fluctuation for the ideal gas in thermodynamic limit is known, the same for both repulsive and attractive interacting BEC is focused in my study. This is a totally unknown field to be explored through an exact many-body method by going beyond mean-field calculation.

### 6.1 Energy fluctuation formulae

## 6.1.1 Energy fluctuation formulae for thermodynamic limiting case

We calculate the full energy spectrum of  ${}^{87}Rb$  and  ${}^{7}Li$  condensates by utilizing the CPHEM method. Average energy for N = 1000 bosons both for  ${}^{87}Rb$  atoms in JILA trap [3] and  ${}^{7}Li$  atoms in RICE trap [4] are calculated. For comparison, we also calculate the energy levels for N = 1000 bosons in noninteracting limit. For the ideal Bose gas in the thermodynamic limit analytic treatment exists. In the thermodynamic limit, the average energy for ideal bosons is

$$\frac{E}{N} = 3k_B T \frac{\zeta(4)}{\zeta(3)} \left(\frac{T}{T_c^0}\right)^3,\tag{6.1}$$

where  $T_c^0$  is the critical temperature for ideal bosons defined as

$$(k_B T_c^0)^3 = \frac{N}{C\Gamma(3)\zeta(3)},$$
 (6.2)

where  $C = \frac{1}{2\hbar^3\omega^3}$ . For  $T > T_c^0$ , as the Bose-Einstein distribution reduces to Boltzmann distribution, the average energy of the condensate becomes

$$\frac{E}{N} = 3k_B T. \tag{6.3}$$

The fluctuation in energy per particle at  $T < T_c^0$  is defined as [85, 93]

$$\Delta E^{2} = (k_{B}T)^{2} \left[ 12 \frac{\zeta(5)}{\zeta(3)} \left( \frac{T}{T_{c}^{0}} \right)^{3} - 9 \left( \frac{\zeta(4)}{\zeta(3)} \right)^{2} \left( \frac{T}{T_{c}^{0}} \right)^{6} \right].$$
(6.4)

The fluctuation in energy at  $T > T_c^0$  can further interpreted as  $\Delta E^2 = k_B T^2 C_v$ . Where  $C_v$  is the specific heat per particle.

## 6.1.2 Energy fluctuation formulae for finite number of particles

The occupation probability of the energy level  $E_{nl}$  is

$$P(E_{nl}) = \frac{f(E_{nl})}{N}.$$
(6.5)

where  $f(E_{nl})$  is the Bose-Einstein distribution function. In the condensate, the average energy of a particle at a temperature T is

$$< E(N,T) > = \sum_{n=0}^{\infty} \sum_{l=0}^{\infty} E_{nl} P(E_{nl})$$
  
 $= \sum_{n=0}^{\infty} \sum_{l=0}^{\infty} \frac{(2l+1)f(E_{nl})E_{nl}}{N}.$  (6.6)

At temperature T, the average of the square of the energy is

$$\langle E^{2}(N,T) \rangle = \sum_{n=0}^{\infty} \sum_{l=0}^{\infty} E_{nl}^{2} P(E_{nl})$$
$$= \sum_{n=0}^{\infty} \sum_{l=0}^{\infty} \frac{(2l+1)f(E_{nl})E_{nl}^{2}}{N}.$$
(6.7)

The energy fluctuation is calculated from the relation as

$$\Delta E^2 = \langle E^2(N,T) \rangle - \langle E(N,T) \rangle^2 .$$
(6.8)

Thus for interacting bosons of finite numbers, we numerically calculate the average energy  $\langle E \rangle$ , energy fluctuation ( $\Delta E^2$ ) and relative energy fluctuation ( $\frac{\Delta E}{\langle E \rangle}$ ) following Eq. 6.6 to Eq. 6.8 [85, 93].

#### 6.2 Effect of interaction on average energy

In figure 6.1, we present the average energy per particle  $\frac{E}{Nk_BT_c^0}$  as a function of reduced temperature  $\frac{T}{T_c^0}$  for repulsive and attractive condensate. Comparison is made with the noninteracting finite sized as well as thermodynamic limiting case. The effective interaction is determined by the parameter  $|Na_s|$ . The scattering length for<sup>87</sup>Rb is 100 Bohr and the same for <sup>7</sup>Li is -27.3 Bohr. Thus for <sup>87</sup>Rb atoms the effective repulsion is stronger than that of <sup>7</sup>Li atoms because the scattering length is large for the former system. The particles are pushed into higher energy states, as the repulsive interaction among the atoms dominates. So, the average energy of <sup>87</sup>Rb condensate is higher than that of <sup>7</sup>Li condensate where due to attraction between the particles the lowest energy state is occupied. Thus, average energy curve for attractive BEC is lower than that of repulsive condensate. At the transition temperature all the average energy curves exhibit a kink which signifies the transition from dilute condensate to classical Bose gas. At  $T > T_c^0$ , all the



Figure 6.1: Plot of average energy  $\frac{E}{Nk_BT_c^0}$  for attractive and repulsive interacting bosons with N = 1000. The energy for the noninteracting bosons and the thermodynamic limit are also presented for comparison.

particles in the condensate move to the excited states, average energy tends to follow the classical value determined by the Eq. 6.3.

# 6.3 Effect of interaction on the energy fluctuation

The effect of interaction on the energy fluctuation  $\frac{\Delta E^2}{k_B^2 T^2}$  is presented in figure 6.2. All four fluctuation curves gradually increase with increase in the temperature, at the transition temperature they attained the maximum value, then drop. At  $T > T_c^0$ , all the fluctuations measure follow the classical limit  $\frac{C_v}{k_B} = 3.0$ . The hump in the energy fluctuation curve for the <sup>87</sup>Rb condensate shifts slightly towards left with respect to the noninteracting curve due to repulsive interaction. However, as the sharpness of the hump in the fluctuation is not very sharp the condensate is far from the possibility of any phase transition for such mesoscopic regime. In an earlier calculation for the same system it has been demonstrated that for repulsive condensate to achieve the phase transition, the number of particles should be truly very large [44]. However, our present calculation is for mesoscopic condensate with a fixed number of bosons. Our motivation is to extract the effect of interatomic interaction and interatomic correlation in the fluctuation measures. So, only the possibility of quasi phase transition is expected. For  $^{7}Li$  condensate, the hump in the fluctuation measure is right shifted, comparing with the case of repulsive as well as noninteracting condensate. In the attractive one, the shift of the hump is quite significant. As the effective interaction  $(|Na_s|)$  is stronger for the repulsive case compared to the attractive interaction so the distinct hump at the transition temperature is solely attributed with the strong interatomic correlation in the attractive condensate. For  $^{7}Li$  condensate as the critical number of particles for the collapse is 1400, we can not compute the fluctuation for a larger number of  $^{7}Li$ atoms in the trap. Second order phase transition is clearly evident from the distinct hump in the thermodynamic limiting curve. The hump sharply decreases for finite sized noninteracting condensate. The shallow peak in the curve is a signature of the possibility of transition from the condensate to the classical Bose gas only. For mesoscopic interacting systems, only quasi phase transition is predicted.



Figure 6.2: Energy fluctuation  $\frac{\Delta E^2}{k_B^2 T^2}$  for attractive and repulsive interacting bosons with N = 1000. The energy fluctuation for the noninteracting bosons and the thermodynamic limit are also presented for comparison.

However, in the present day experiment the interaction strength  $a_s$  is tunable

through the Feshbach resonance [154]. As critical stability factor is determined by  $k_{cr} = \frac{N_{cr}|a_s|}{a_{ho}}$ , it is possible to set up suitable attractive condensate which can accommodate large number of bosons before collapse. It will facilitate to measure fluctuation at the transition temperature for a larger number of attractive bosons. Thus, our observation made in figure 6.2 can be verified experimentally in future experiment. We conclude that the dilute condensate in the mesoscopic regime exhibits the same physics qualitatively irrespective of the type of interaction. However, the significant difference in fluctuation measures in attractive condensate compared to the repulsive as well as noninteracting case clearly establish the effect of interatomic correlation.

# 6.4 Effect of interaction on relative energy fluctuation

Next, we study the relative fluctuation for repulsive and attractive condensate in figure 6.3 and the comparison is done with noninteracting case. We observe drastic effect of both repulsive and attractive interactions in the measure of relative energy fluctuation. We see from the energy fluctuation curve  $[\Delta E^2, \text{ figure 6.2}]$  that fluctuation is almost the same for the both kind of interacting and noninteracting condensate. But the change in the average energy is large  $[\langle E(N,T) \rangle$ , figure 6.1]. The relative fluctuation  $(\frac{\Delta E}{\langle E \rangle})$  is a ratio between the above two quantities -the average energy and energy fluctuation. Thus, overall effect in relative fluctuation is significant for the attractive BEC since the change in average energy for  $^7Li$  is large near the transition temperature  $(T_c)$ .

#### 6.5 Three characteristic temperatures

For ideal Bose gas in the thermodynamics limit, the different thermodynamic functions and the condensate fluctuation exhibit true singularity at the transition temperature. The transition temperature is taken as the characteristic temperature which corresponds to phase transition. However, for the finite sized system as we found the fluctuation measures only exhibit maxima at the transition temperature



Figure 6.3: Plot of relative energy fluctuation  $\left(\frac{\Delta E}{\langle E \rangle}\right)$  for attractive and repulsive interacting bosons with N = 1000. The relative energy fluctuation for the noninteracting bosons is also presented for comparison.

- the point of maximal fluctuation can be taken as the definition of characteristic temperature. Characteristic temperatures are defined by several authors in some earlier works [107, 155, 156, 157, 158]. It can be defined as the inflexion point in the ground state occupation probability distribution of the condensate. Alternatively one can define the characteristic temperature from the maxima in In our present work, we stress the possibility of other charthe specific heat. acteristic temperatures calculated from the energy fluctuations. We define three characteristic temperatures calculated from the maximal fluctuations of average energy, energy fluctuation and relative energy fluctuation. They are respectively denoted by  $T_m^{AE}$ ,  $T_m^{EF}$  and  $T_m^{RE}$ , choices of abbreviation are as follows : AE  $\rightarrow$ average energy,  $EF \rightarrow energy$  fluctuation and  $RE \rightarrow relative energy$  fluctuation. In figure 6.4 we plot the variation of these characteristic temperatures as a function of interaction strength  $Na_s$ . All the graphs smoothly change as a function of interaction strength. However, it is also instructive to calculate the characteristic temperature for various N values and to study their behaviour at large particle number limit. For attractive condensate, due to quick collapse we are unable to



Figure 6.4: Plot of characteristic temperatures  $\frac{Tm}{T_c^0}$  as a function of scattering length  $a_s$ . Detailed discussion of  $T_m$  is given in the text.



Figure 6.5: Plot of characteristic temperatures  $\frac{Tm}{T_c^0}$  against the number of particles N for repulsively interacting <sup>87</sup>Rb atoms in the harmonic trap. Detailed discussion of  $T_m$  is given in the text.

calculate energy fluctuation beyond N = 1000. However, for repulsive condensate we calculate  $T_m^{AE}$ ,  $T_m^{EF}$  and  $T_m^{RE}$  in the unit of  $T_c^0$  for N = 500, 1000, 5000, 7000 and 11000. In figure 6.5, we plot them as a function of N. All characteristic temperatures will tend to the critical temperature defined in the thermodynamic limit.