Chapter 10

Summary and conclusion

The key motivation of our work is to present an *ab initio* many-body calculation of thermal fluctuations for weakly interacting dilute bulk BEC and an exact time-dependent many-body calculation to study highly correlated, strongly interacting few-bosonic systems.

The first part of this thesis is focused to study the statistical fluctuations and thermodynamic properties for the trapped interacting Bose gases by utilizing an exact many-body calculation. We have considered real experimental scenario and beyond the mean-field calculation of several thermodynamic and statistical properties are presented here. Experimental realization of atom number fluctuation for the dilute weakly interacting BEC [144] motivated us to study several statistical fluctuations in interacting BEC in detail. We have presented a complete study and probably the first study of condensate statistics and statistical fluctuation of attractive Bose gas in three dimensional harmonic trap. We utilize the two-body correlated basis function to describe the N particle Hamiltonian. The interatomic interaction is taken as van der Waals interaction. We consider ^7Li atoms with scattering length $a_s = -27.3 \pm 0.8$ Bohr which mimics the Rice University experiment [4]. The critical number of atoms for the collapse for ^7Li condensate is around $N_{cr} = 1400$. Thus, ^7Li is truly mesoscopic system and an ideal platform to calculate several condensate statistics and fluctuations. In the context of recent experimental findings, it is known that the trap geometry has very strong influence on the stability of BEC, evolution of atomic cloud, energy of the particles, specific heat and several fluctuation properties like condensate fraction, central moments. So, not only the simple harmonic oscillator trap of infinite extent we consider anharmonic trap of finite extent which plays a major role to describe the stability of the condensate. Statistical fluctuation of repulsive interacting ^{87}Rb atoms in anharmonic trap is our center of attraction. Also the energy fluctuation phenomenon in BEC and the effect of repulsive as well as attractive interaction on the energy fluctuation have also been studied. All these calculations have been performed by an approximate many-body method CPHEM which facilitates the effect of interparticle interaction as well as finite size. All two-body correlations were included to go beyond the mean-field GP equation.

We discussed the thermal evolution of condensate fraction for attractive interacting ^{7}Li condensate and it exhibits the depletion of the condensate with increase in temperature. We have calculated the root-mean-square fluctuation and see that it smoothly passes near the critical temperature. However, near $T = T_c^0$ we observe the effect of truly finite size. We also report the condensate fluctuation as a function of reduced temperature T/T_c^0 and negative interaction strength parameter Na_s. The external confinement reduces the thermal fluctuation, unlike the uniform Bose gas where thermal fluctuation may destabilize the condensate. Thus, the sharp fall in the standard deviation and several orders of central moment near the transition temperature exhibit the effect of finite size system.

We have calculated statistical fluctuations in the canonical ensemble for the trapped repulsive interacting ^{87}Rb condensate in a harmonic trap and also in a very tight trap. We observed that the transition temperature increases in the tight trap which makes favourable condition to achieve BEC. Study of the lambda-structure in different measures of fluctuation (standard deviation, several orders of central moment) near the transition temperature is also interesting. Although all the measures in anharmonic trap are clearly distinguishable from those in the harmonic trap, the essential lambda-structure near the transition temperature remains the same qualitatively. We defined three possible characteristic temperatures from the location of inflexion point of the lambda-structures. We observe all the fluctuations curves gradually increase with increase in anharmonicity which further confirms that a strong anharmonic trap favours BEC. However, from similar qualitative behavior of all the statistical measures near the transition temperature, it may be concluded that the mesoscopic BEC exhibits quasi phase transition. To confirm this quasi phase transition for the mesoscopic BEC, we further calculate the transition exponent using the specific heat capacity. It shows that the exponent sharply changes near the transition temperature in a harmonic trap and thus quasi phase transition is more prominent in the harmonic trap in comparison with the anharmonic traps.

The energy fluctuation and especially the effect of interaction on the several measures of energy fluctuations did not receive much attention till yet. Here we presented the energy fluctuation measures considering the experimental parameters of ^{87}Rb atoms in JILA trap and ^{7}Li atoms in RICE trap. By observing the nature of the energy fluctuation curves the possibility of phase transition in mesoscopic regime can be simply ruled out both for attractive as well as repulsive condensate. For repulsive BEC as the condensate is always stable, the thermodynamic limit can be achieved. For the attractive BEC as the condensate always collapses with small number of bosons, it is always mesoscopic. Unlike repulsive BEC, which is less correlated, the attractive BEC is strongly correlated even in the mesoscopic regime. Thus, our findings are important in few ways. The mean-field theory is not suitable to discuss the correlated BEC and thus unable to calculate the fluctuation measures reported in this work. In our knowledge, this is the first theoretical calculation of energy fluctuation measures of attractive condensate which can be measured in future experiments. We also define several characteristic temperatures from the point of maximal fluctuation of the energy fluctuations and their dependence on the particle number and interaction strength. All the characteristic temperatures smoothly approach the critical temperature limit for a quite large number of bosons in the trap.

The key motivation of the second part of this thesis is to study the process of fragmentation and also the continuous phase transition from condensed superfluid (SF) to fragmented Mott insulating (MI) phase. The pathway from the condensed phase (single-orbital is populated) to fragmented phase (higher orbitals are also populated) has been discussed which is beyond the scope of any mean-field approach. How the continuous phase transition in an optical lattice can be studied by observing the evolution of one- and two-body density, Shannon information entropy and first- and second-order correlation function have been presented. The link between the loss of first-order coherence and Shannon information entropy has been studied in great detail. The effect of long-range dipolar interaction on the correlation functions and entropy production are presented. The collapse - revival process in lattice depth quench process is related to the phase diffusion due to the quantum fluctuation. How the atom number fluctuation, arising due to the quantum fluctuation, in reduced dimensional systems depends on contact as well as on dipolar interaction are discussed.

In such strong interacting regime the system gets fragmented and we observe smooth transition from the condensation to fragmentation with the continuous increase in the interaction strength. Several new intriguing phases emerges in reduced dimension. We highlight the key characteristics of the many-body wave function that reveal the difference between the fermionized bosons with contact interaction and crystallized bosons with dipolar interaction. In the case of fermionization, the one- and two-body density shows a modulation with a number of maxima corresponding to the number of particles. The maxima are confined but not completely separated. The incomplete separation is a consequence of the representability of momentum distribution of fermionized bosons using a basis set: infinitely many basis states are necessary to accurately resolve the cusp – a fact that is reflected by the depletion of the state which we quantified by the eigenvalues of the reduced one-body density matrix. In the case of crystallization, the one- and two-body density show well-separated peaks whose distances diverge as a function of the interaction strength. This complete separation is the consequence of the formation of a Mott-insulator-alike many-body state where the "lattice potential" is replaced by the long-ranged interparticle interactions and the "lattice constant" is dictated by the strength of the interparticle interactions. It is to be noted that all the signatures that distinguish crystalline bosons from fermionized bosons can be measured experimentally using single-shot absorption imaging [175, 176, 177, 178, 179]. From experimental absorption images, the one-body and two-body density are available as averages of many single-shot images. Thus, a direct verification of our results for the spread of the one-body and two-body density can be performed. Furthermore, Refs. [173, 180] suggest that the natural occupations can be inferred from the integrated variance of single-shot images, at least at zero temperature.

We also study the quench dynamics of 1D interacting bosons in an optical lattice from the first principle general quantum many-body perspective using the MCTDHB method covering both the significantly strong interactions and the shallow optical lattice. We observe that the dynamics of the two different quenches show significantly different behavior from each other. For strong interaction quench, the system enters the MI phase on a small timescale and the system relaxes to that maximum entropy state. The relaxation process is observed through the time evolution of the natural occupations, entropy evolution, and the reduced density matrices. The relaxation time follows a power law decay with respect to the interaction strength. In contrast, for the lattice depth quench with the same excitation energy, the MI phase is reached on a very long timescale, significantly larger compared to the interaction quench. For the lattice depth quench, the system does not relax and exhibits a collapse-revival dynamics in the long timescale which is revealed in all the computed measures. The corresponding revival time exhibits a power law decay with respect to the lattice depth parameter. As per our knowledge, in these two independent quench processes (interaction quench and lattice depth quench), estimation of the timescale of relaxation and revival and their connection with entropy production are not reported earlier. Our theoretical investigation of quench dynamics tuning the parameters related to microscopic Hamiltonian can be verified in future experiments.

We studied the quench dynamics of 1D dipolar bosons in a triple-well optical lattice from the first principle general quantum many-body perspective utilizing the MCTDHB method for both shallow and deep optical lattices. The comparison with the contact interaction is also presented. For forward lattice depth quench for both the contact and dipolar interaction, we observe collapse–revival dynamics in the time evolution of normalized first-order Glauber's correlation function. The observed dynamics is further linked with the production of many-body Shannon information entropy. However, both the collapse and revival time reported for dipolar interaction are significantly smaller than those corresponding to the contact interaction. The quantum collapse-revival dynamics observed for lattice depth quench in 1D optical lattice shows how the atom number fluctuation varies during the quench process. The on-site atom number fluctuations can be probed by measuring the ratio of collapse time $t_{collapse}$ to revival time $t_{revival}$. We characterized $\tau = \frac{t_{collapse}}{t_{revival}}$ as the figure of merit to reflect the width of the atom number distribution [83]. This figure of merit is independent of the depth of the lattice potential which concludes that atom number fluctuation is also independent of the depth of the lattice potential. τ for the contact interaction lies within the same band as depicted for dipolar interaction. This observation is in agreement with previous experimental results (figure 2 of Ref. [83]) where the initial atom number distribution was considered as Poissonian and the width of the fluctuation was calculated.

In future we want to sudy effect of long range interaction on the transition temperature of mesoscopic BEC. Collective excitation of the weakly interacting system in anharmonic trap is also an open direction to study. Presently I am studying the quench dynamics for several long-range interactions and expecting to observe new intriguing phases when the range goes below the dimension of the system.