Chapter 7

Fragmentation of BEC in harmonic trap

In the previous few chapters, we have discussed about the quasi phase transition through the study of different thermodynamic properties like condensate fraction, atom number fluctuation, several orders of central moment and specific heat, etc. of the bulk interacting BEC. However, only weakly interacting dilute BEC was considered. The time-independent Schrödinger equation was numerically solved by a many-body method CPHEM. The bulk statistical properties were reported but not the exact many-body physics was discussed. The emergence of the recent experiments with few bosons both in harmonic trap and optical lattice proved that huge effect over several static and dynamical properties are coming from the strong interatomic interaction, dimensionality of the system and trap geometry [45, 46, 73, 74, 75, 76, 77, 78, 79, 80]. Even at the zero temperature due to quantum fluctuation continuous phase transition from condensed superfluid (SF)to fragmented Mott insulating (MI) phase may happen in reduced dimension. By utilizing MCTDHB method we can calculate exact quantum many-body dynamics for a few numbers of strongly interacting trapped bosons. By this exact many-body method we can go beyond the single particle mean-field approximation and can handle strongly interacting as well as highly correlated systems. For the present purpose, we will consider few interacting bosons trapped in a 1D harmonic oscillator (HO) and also in an optical lattice (OL). The time-dependent Schrödinger equation is solved numerically to study the phase transition. The loss of coherence, build up of correlation and emergence of information entropy for few strongly interacting bosons are associated with the fragmentation and phase transition process. The study of these key quantities have now become very interesting and challenging research area. For the few-particle system, not the statistical fluctuation but the atom number fluctuation is the key quantity to be studied. The exact many-body method applied for the study of few boson system has enormous control over almost all the system parameters like the interaction strength, lattice depth and trap geometry. By changing these parameters of the many-body Hamiltonian we can study the evolution of several physical quantities like one-body density, two-body density and natural occupations to study the fragmentation and phase transition process.

The density profile for the trapped interacting bosons in a harmonic oscillator with both contact and dipolar interaction is numerically investigated at a manybody level from first principles. In the mean-field Gross-Pitaevskii theory, the total wave function is considered as a simple product of many single particle states. So, the reduced density matrix has only one eigenvalue for any time. Only one-lowest quantum state is occupied producing a single-peaked wave function for every time. This basically corresponds to the fact that, the system remains condensed for all the time never fragments i.e., the particles never occupy any higher excited state. The contrast physics can be seen from several theoretical and experimental works when the interparticle interaction is very strong. Different new phases like fermionization in contact interacting system appear [166, 167, 168, 169, 170, 171]. By utilizing MCTDHB method, one can study the pathway from the condensed phase to fragmented phase. From the many-body wave function $\psi(x_1, x_2, ..., x_N; t)$, the one-body reduced density matrix (RDM) $\rho^{(1)}$ can be calculated as

$$\rho^{(1)}(x'|x;t) = N \int dx_2 dx_3 \dots dx_N \psi^*(x', x_2, \dots, x_N;t)$$

$$\psi(x, x_2, \dots, x_N;t).$$
(7.1)

The diagonal elements of RDM constitute the one-body density, $\rho(x, t)$, as

$$\rho(x,t) = N \int dx_2 dx_3 \dots dx_N \psi^*(x, x_2, \dots, x_N; t) \psi(x, x_2, \dots, x_N; t)$$
(7.2)

and give the probability of a particle at the position x at time t when the contribution of other particles are traced out. The non-local correlations are determined by the off-diagonal kernel of $\rho^{(1)}(x'|x;t)$. When $|x - x'| \to \infty$, the off-diagonal behavior of $\rho^{(1)}(x',x)$ measures the coherence. One of the key measures to assess the degree of condensation & coherence or fragmentation & incoherence is the natural occupations. The natural occupation and the orbitals of the system are the eigenvalue and eigenfunction of the reduced one-body density matrix. The population in the higher natural orbitals are the signature of the emergence of fragmentation from the condensate. The two-body reduced density matrix is defined as

$$\rho^{(2)}(x_1', x_2'|x_1, x_2; t) = N(N-1) \int dx_3 dx_4 \dots dx_N$$

$$\psi^*(x_1', x_2', x_3, \dots, x_N; t) \psi(x_1, x_2, \dots x_N; t)$$
(7.3)

Its diagonal kernel can be written as

$$\rho^{(2)}(x_1, x_2; t) \equiv \rho^{(2)}(x_1' = x_1, x_2' = x_2 | x_1, x_2; t)$$
(7.4)

and represents the simultaneous probability of finding a boson at x_1 and another at x_2 .

7.1 Identification of Fermionization and Crystallization

Depending on the interaction strength, the bosons trapped in a harmonic oscillator show different phases - starting from condensed phase to fragmented phase. In the former phase, only one natural orbital is macroscopically occupied and with increase in interaction strength several other higher orbitals start to be populated -fragmentation occurs. Fermionization for bosons occurs when they feel an infinite repulsive contact interaction in one spatial dimension. For fermionized bosons, the total energy E and the density [Eq. (7.1)] of the system become exactly equal to the energy and the density of non-interacting spin-less fermions respectively. For our few-bosons system (N = 4) in a harmonic trap with frequency one, $V(x) = \frac{1}{2}x^2$, the limiting value of energy is thus $E_{\lambda \to \infty}^{N=4} = 8.0$ [see figure 7.1]. As fermionization occurs for bosons with contact interaction, crystallization occurs for bosons with dipole-dipole interaction - when the long-range tail of the interaction (Eq. (2.37)) becomes dominant. The bosons form a lattice structure which allows them to minimize their mutual spatial overlap. Unlike the fermionization, the energy does not saturate for crystallized bosons - it is unbounded. From fitting the energy in figure 7.1, we can infer that the energy as a function of contact interaction strength approaches the fermionization limit exponentially. For dipolar interaction, the growth of the energy as a function of the interaction strength is fitting well to a power law figure 7.1. To characterize fermionization and crystallization we analyze the one- and two-body density for bosons with both contact and dipolar interaction respectively. Also, the fully fragmented states of bosons with contact interaction (fermionization) and with dipolar interaction (crystallization) can be understood by observing the population in the natural orbitals.



Figure 7.1: Tracing fermionization and crystallization by the evolution of the energy.

7.1.1 Fragmentation with contact interaction : Fermionization

We start our investigation with the study of one-body density as a function of interaction strength λ , for the N = 4 harmonically trapped bosons [see figure 7.2]. Bosons are interacting through contact delta interaction. The form of trapping potential and the interaction potential are given in the methodology Chapter 2.2. For comparatively weak repulsion, the density is clustered at the center of the trap and becomes flatter and broader when λ increases. For stronger repulsion, the density gradually acquires modulations and the number of humps finally saturate to the number of bosons in the system; four humps for N = 4 bosons are clearly visible when the interaction strength becomes $\lambda \sim 10$. The emergence of equal number of maxima in the density as the number of bosons indicates that the Tonks-Girardeau (TG) regime is approached. The density modulations/humps are more pronounced in the center of the trap, where the potential is close to zero. For larger distances from the trap center, the humps in the one-body density profile are less pronounced due to the non-zero value of the confining potential. It is to be noted that, the maxima in the density in the Tonks-Girardeau regime are distinct but not isolated. We also observe that, once the TG regime is reached, the density does not broaden further with increasing values of λ .

Next, we move to discuss the two-body densities $\rho^{(2)}$ of bosons with contact interaction. For weak interaction strength, $\lambda = 0.1$, the bosons are clustered near the center at $x_1 = x_2 = 0$. As the interaction strength λ increases, $\rho^{(2)}$ spreads out to the off-diagonal $(x_1 \neq x_2)$ while the diagonal $(x_1 \sim x_2)$ is depleted as shown in figure 7.3(a) for $\lambda = 1$. For stronger repulsions ($\lambda = 10$ and $\lambda = 30$), a correlation hole in the two-body density ($\rho^{(2)}(x, x) \rightarrow 0$) forms on the diagonal. This basically means that the probability of finding two bosons at the same position (along the diagonal) tends towards zero. In the limit of infinite repulsion, the correlation hole persists in the two-body density $\rho^{(2)}$. With increase in the interaction strength, not only the density, but also the energy of fermionized bosons saturates to the energy of non-interacting fermions. In analogy to the boundedness of the energy as a function of the interaction strength, the width of two-body density on its anti-diagonal [$\rho^{(2)}(x, -x)$] is also bounded, i.e., the spread of $\rho^{(2)}$ converges in the



Figure 7.2: One-body density of four bosons as a function of contact $[(\mathbf{a}), (\mathbf{b})]$ and dipolar $[(\mathbf{c}), (\mathbf{d})]$ interparticle interaction strength. For contact interaction, the density becomes flatter and broader as the repulsion increases [panel (**a**), (**b**)]. For larger interaction strengths $[\lambda \gtrsim 10]$ four distinct but not isolated peaks appear and the density gradually converges to the density of four non-interacting fermions as $\lambda \to \infty$. Due to this convergence, the spread of the density seizes to increase fermionization emerges. For dipolar interaction, the one-body density is clustered at the center of the trap for small interactions [panels (**c**),(**d**) for $g_d \leq 1$]. As g_d increases(≥ 1) the density develops a fourfold splitting. As a function of increasing interaction strength, the spread of the density continues to increase [panel (**d**)] and the fourfold spatial splitting intensifies to form four completely isolated peaks in the density for sufficiently strong dipolar interaction - crystallization emerges for $g_d \gtrsim 10$. All quantities shown are dimensionless.

fermionization limit when $\lambda \to \infty$. Similar to the one-body density, the maxima which are formed in the off-diagonal of the two-body density are distinct but not isolated [see figure 7.3(a) for $\lambda = 10$ and $\lambda = 30$]. We infer that the correlation hole along the diagonal and the confined spread are the unique signatures of the two-body density of a fermionized state.

7.1.2 Fragmentation with dipolar interaction : Crystallization

To distinguish between fermionization and crystallization phases, we will analyze the one-body and two-body density of the bosons interacting with dipolar interaction. We start the analysis, by plotting the one-body density of N = 4 bosons as a function of dipolar interaction strength (g_d) as depicted in figure 7.2(c) and (d). The system is condensed at the center of the trap for small $g_d \sim 0.1$. As g_d increases $(g_d \in 1, \infty 5)$, the density starts to exhibit a four-hump structure as depicted in figure 7.2(c) and (d). This *attempted fermionization*, results from a dominant contribution of the short-range part of the dipolar interaction potential [170]. However, this fermionization-like behavior is only a precursor to the crystal transition that takes place when the long-range nature of the interaction starts to dominate the physics of the system for larger interaction strengths with $g_d \gtrsim 10$. At $g_d = 30.0$, we observe four *well-isolated* peaks heralding the crystallization of the N = 4 bosons.

We now move to analyze, the behaviour of the two-body density of trapped bosons for dipole-dipole interaction in figure 7.3(b). For small interaction strength, $g_d = 0.1$, the bosons are clustered together at the center of the trap. As g_d increases ≥ 1 , a correlation hole develops: $\rho^{(2)}(x, x)$ tends to zero as shown in figure 7.3(b). Thus, the probability of finding two bosons in the same place (along the diagonal) is strongly reduced due to the long-range interaction. In the crystalline phase for $g_d \geq 10$, the bosons escape their spatial overlap entirely and even the off-diagonal peaks of $\rho^{(2)}$ become isolated. We term this behavior as the emergence of an offdiagonal correlation hole. For crystallized bosons, the spread of the anti-diagonal of the two-body density, $\rho^{(2)}(x, -x)$, is diverging as g_d is increasing. This can be inferred by comparing the spreading of the anti-diagonal for $g_d = 10$ to $g_d = 30$. We assert that the correlation hole along the diagonal and the off-diagonal and the unbounded spreading are the unique signatures of the two-body density of a crystalline state of dipolar bosons.



Figure 7.3: Two-body density of four bosons as a function of contact $[(\mathbf{a})]$ and dipolar $[(\mathbf{b})]$ interparticle interaction strength. For contact interaction, the atoms are clustered at the center $(x_1 = x_2 = 0)$ for small interaction strengths for $\lambda = 0.1$. As λ increases (> 1), the two-body density starts to spread due to the repulsion between the bosons. For stronger interaction strengths, $\lambda = 10$ and 30 the diagonal of $\rho^{(2)}(x, x)$, is practically 0: the bosons completely avoid their spatial overlap and a "correlation hole" develops. For dipolar interaction, the atoms cluster at the center $(x_1 = x_2 = 0)$ for small interaction strengths for $g_d = 0.1$. As g_d increases (≥ 1) , the diagonal part, $\rho^{(2)}(x, x)$ starts to be depleted because the long-range interactions start to dominate the physics. At stronger interaction strengths, the diagonal correlation hole spreads, i.e., the area in the vicinity of $x_1 \approx x_2$ for which $\rho^{(2)}(x_1, x_2) \approx 0$ holds is enlarged as a function of g_d . For dipolar interaction contrast behaviour from contact interaction is evident - the off-diagonal $(x_1 \neq x_2)$ of $\rho^{(2)}(x_1, x_2)$ forms a complete correlation hole, compare panel (a) for $\lambda = 30$ and panel (b) for $g_d = 30$. All quantities shown are dimensionless.

7.2 Fragmentation in terms of natural occupation

We now start analyzing the eigenvalues of the reduced one-body density matrix, the so-called natural occupations [172], as a function of the interaction strength between the particles [figure 7.4(a)–(b)]. As expected [163, 173, 174], when the value of the interaction strength increases, the occupation of the first natural orbital decreases while the other orbitals start to be populated. For contact interaction, mostly one natural occupation, n_1 , dominates for the whole interaction regime starting from very small λ . While the other occupations $n_k, k > 1$ remain comparatively small even for large values of λ . When λ is very large the depletion in the occupation emerges as the fermionized state is reached as depicted in figure 7.4(a).



Figure 7.4: Tracing fermionization and crystallization by the evolution of the natural occupations [panel (a) and (b)] as a function of the interaction strength. The eigenvalues of the reduced density matrix, i.e., the natural occupations $\rho_i^{(NO)}$ exhibit depletion for contact interaction (many small $\rho_i^{(NO)}$ with i > 1 emerge) and full-blown N-fold fragmentation for dipolar interaction (all $\rho_i^{(NO)}$ with $i \leq N$ contribute equally). The $\rho_i^{(NO)}$ have organized in decreasing order starting from i = 1. All quantities shown are dimensionless.

For dipole-dipole interaction, when the interaction strength g_d is very small

then only the first orbital is occupied showing condensation. Fragmentation starts with the increase in the interaction strength. However, for long-range interaction, all occupations $\rho_k^{(NO)}$ for $k \leq N$ contribute on an equal footing for large values of g_d . This full-blown N-fold fragmentation emerges as the crystal state is reached [figure 7.4(b)]. The emergence of complete fragmentation is a consequence of longranged interaction and in sharp contrast to the emergent depletion in the case of contact interaction.