### Chapter 8

## Statistical relaxation of few strongly correlated bosons in optical lattice

The simplest non-equilibrium process is the quantum quench where the system is driven out of equilibrium by changing any parameter of the Hamiltonian abruptly [59, 60, 61, 181, 182, 183, 184, 185, 186, 187, 188, 189, 190, 191]. Remarkable experimental progress with ultracold trapped gases triggered the study of nonequilibrium dynamics of isolated quantum systems [45, 46, 73, 74, 75, 76, 77, 78, 79, 80]. Bosons trapped in an optical lattice is an isolated quantum many-body system which offers enormous control over several system parameters. The interaction strength, lattice depth and trap geometry can be easily adjusted to bring the system out-of-equilibrium. Due to quench, a continuous phase transition from superfluid (SF) to Mott insulator (MI) phase emerges in the optical lattice. By observing the time dynamics of correlation functions and entropy evolution of the quenched system, we can understand the many-body physics. In the superfluid phase, full coherence over the whole lattice is observed and both inter- and intrawell tunneling of bosons are allowed. In the Mott insulating phase, individual bosons occupy a single site of the lattice by diminishing the inter-well tunneling.

The one-body and two-body density of trapped interacting bosons in a triple well optical lattice are investigated numerically on a many-body level from first principles. The coherence properties are analyzed. A generic fragmentation scenario of a condensate is considered. The density profiles are showing the pathway from a condensed superfluid to a fragmented Mott insulator phase. Full coherence is related to the SF phase and loss of coherence is related to the fragmented MIphase. The connection between the evolution of Shannon information entropy and loss & gain of coherence are discussed. The system may relax to a maximum entropy state or can oscillate between the minimum and maximum value depending on the quench process. To explore the process of the continuous phase transition from condensed (SF) to fragmented (MI) phase, by observing the change in the above mentioned physical quantities around the transition point, we perform two-kind of quenches : interaction quench and lattice depth quench.

# 8.1 Interaction strength quench and lattice depth quench

Our setup consists of N = 3 bosons in a one-dimensional triple well (S = 3) optical lattice. The external lattice potential with periodic boundary condition is modeled as  $V_{OL}(x) = V \sin^2(kx)$  with V being the lattice depth and k the latticewave-vector. By quenching any parameter of the Hamiltonian, one can study the phase transition of the system from SF to MI. We quench the system by changing the interaction strength  $(\lambda)$  suddenly by keeping the lattice depth (V) fixed - this is termed as interaction quench. We also study the lattice depth quench where we instantaneously change the lattice depth by keeping the interaction strength fixed. Time evolution of several measurable quantities like one-body and two-body density and Shannon information entropy have been observed.

The one- and two-body density can be calculated by the formulas already discussed in Chapter 7.1. In position space, the Shannon information entropy (SIE) of the one-body density is defined as  $S_x(t) = -\int dx \rho(x,t) ln[\rho(x,t)]$ . Similarly in the momentum space, it can be defined as  $S_k(t) = -\int dk \rho(k,t) ln[\rho(k,t)]$  [205, 206]. The two SIEs as defined above are two independent key quantities in the calculation of quantum information in many-body system. The SIEs are the measure of the delocalization of the corresponding distributions. However, as SIEs are calculated by utilizing the one-body density, one can not infer the presence of correlation in the many-body state. Whereas in MCTDHB, as the many-body wave function is expanded in the time-dependent coefficients as well as time-dependent orbitals, we, therefore provide alternative definitions of SIE. The SIE defined from the coefficients  $C_{\bar{n}}$  is called information entropy or coefficient entropy and it is calculated from

$$S^{info}(t) = -\sum_{\bar{n}} |C_{\bar{n}}(t)|^2 \ln |C_{\bar{n}}(t)|^2$$
(8.1)

 $S^{info}$  characterizes the distribution of the many-body state in the underlying Fockspace. The many-body measure of information entropy can be explicitly made by writing the coefficients as expectation values in terms of M creation and annihilation operator [202].

#### 8.1.1 System set up

For the interaction quench, to achieve the superfluid (SF) to Mott insulator (MI)transition, the ground state is prepared with depth V = 3.0 and  $\lambda = 0.1$  initially. Then, keeping V fixed,  $\lambda$  is changed instantaneously to  $\lambda = 15.0$ . This corresponds to pumping the system with energy E = 4.89 through the two-body interaction term in the Hamiltonian. For lattice depth quench, we prepare identical initial state as the interaction quench ( $\lambda = 0.1, V = 3.0$ ) and instantaneously increase the lattice depth to V = 10.1 keeping  $\lambda$  fixed. Since the system is quenched to a higher value of lattice depth from a lower value - it is called forward lattice depth quench. If we quench the system from a higher lattice depth to a lower one then we call it reverse lattice depth quench. Here, the values from the two kinds of quenches (forward lattice depth quench and interaction quench) are chosen such a way that the system is pumped with the same amount of excitation energy E = 4.89 as the  $\lambda = 15.0$  interaction quench. However, as the pumped energy is now distributed as the one-body term in the Hamiltonian, the system responds differently in the dynamics. Depending on the distribution of the supplied energy, the dynamics for the two kinds of quenches become very different. Here, we will study the time variation of natural occupation, one- and two-body density matrix and Shannon information entropy for the above two quench scenarios.



Figure 8.1: (a) Natural occupations as a function of time for interaction quench to  $\lambda = 15.0$ . Computation is done with M = 18 orbitals. The initial condensed SF phase fragments with time and lowest three natural orbitals are occupied. At time t = 1.25, the system becomes fully fragmented MI phase with  $\approx 30\%$ occupation of lowest three orbitals. (b) Natural-orbital occupations as a function of time for lattice-depth quench to V = 10.1. Computation is done with M = 6orbitals. The initial SF phase fragments with time and all three natural orbitals are occupied. At time t = 31.0, the system becomes fully fragmented MI phase with almost 30% natural occupation in three orbitals. In both the occupation plots shown above  $n_2$  and  $n_3$  overlap with each other due to translational invariance. The contribution from all the other higher orbitals are negligible and they almost overlap. All quantities are dimensionless.

Natural orbital occupations  $n_i$  as a function of time for the interaction quench is plotted in figure 8.1(a). Initially, at t = 0, only the first natural orbital contributes, which corresponds to the SF phase, the many-body wave function is condensed, equivalent to the mean-field state, represented as  $|3, 0, \ldots, 0\rangle$ , where the number denotes the population of the corresponding orbitals. With increasing time, fragmentation occurs, and at t = 1.25 the lowest three orbitals exhibit population almost 30%, which is nearly three-fold fragmentation. This three-fold fragmented state  $|1, 1, 1, 0, ..., 0\rangle$  corresponds to the *MI* state. Thus, at time t = 1.25, the system makes a transition from the condensed *SF* to fragmented *MI* phase.

The time evolution of natural occupation for the lattice depth quench is shown in figure 8.1(b). The initial SF state starts to get fragmented and enters the fragmented MI state for the first time at t = 31.0. The required time for fragmentation for lattice depth quench is significantly larger than the time required for the interaction quench to reach fragmented state. This significantly slower  $SF \rightarrow MI$  transition i.e., a larger characteristic time to reach MI phase, distinguishes the lattice depth quench from the interaction quench.

#### 8.3 Time evolution of one-body density

The reduced one-body density matrix  $|\rho^{(1)}(x', x)|^2$  for the interaction quench is depicted in figure 8.2 for different times. Initially, at t = 0, a uniform distribution of maxima are found showing that the initial state (which is SF) displays both intrawell as well as inter-well phase coherence. As time t increases, the off-diagonal maxima fade out and the diagonal contributions become more pronounced. At time t = 1.25, which corresponds to the equivalent MI phase, only the diagonal maxima are observed with a complete absence of the off-diagonal contributions showing a complete absence of phase coherence. From long-time dynamics, we do not observe any revival of coherence and can conclude that the system relaxes. Thus, figure 8.1(a) and figure 8.2 jointly conclude that t = 1.25 is the required time for the system to enter in the MI phase. The complete extinction of the off-diagonal correlation at longtime also supports that the MI phase is retained even for a long time.

The corresponding reduced one-body density matrix for lattice depth quench is presented in figure 8.3 which clearly exhibits a long time collapse-revival dynamics reminiscent of the one observed in the Greiner's experiment [45, 46]. The initial superfluid phase becomes fragmented MI phase at time t = 31.0. At this time inter-well coherence is totally lost only intra-well coherence persists. The phase coherence revives at time t = 81.0 which corresponds to the initial coherent SF



Figure 8.2: Time evolution of the reduced one-body density matrix  $|\rho^{(1)}(x', x)|^2$  for interaction quench  $\lambda = 15.0$ . We observe very fast relaxation to MI phase (see text). All the quantities are dimensionless.

phase.

#### 8.4 Time evolution of two-body density

The two-body density  $\rho^{(2)}(x_1, x_2)$  for interaction quench is shown in figure 8.4. At t = 0.1, the diagonal maxima show a reduction in amplitude compared to the off-diagonal maxima. However, at time t = 1.25, an equal distribution per site is achieved although the diagonal does not extinguish completely. With increasing time, the diagonal contributions fade out, and complete depletion of the diagonal is achieved at a much larger time which sustains for a long time further demonstrating the relaxation process.

The time evolution of the two-body density for the lattice depth quench is presented in figure 8.5. The diagonal maxima are reduced with time and but not completely depleted at the time when the complete depletion of the off-diagonal



Figure 8.3: Time evolution of the reduced one-body density matrix  $|\rho^{(1)}(x',x)|^2$  for lattice-depth quench V = 10.1. The system exhibits revival to the initial phase in the long time dynamics. All the quantities are dimensionless.

coherence is observed in one-body density around t = 31.0. Again, with time, the diagonal coherence increases and revives at long timescale around t = 81.0. So, two-body density also depicts the collapse-revival scenario almost the same as the one-body density.

## 8.5 Time evolution of Shannon information entropy

The study of Shannon information entropy and relaxation of the system are very interesting topics to be discussed. It will also be interesting to study how the entropy evolution is linked with the loss of coherence in one-body density. For interaction quench, the Shannon information entropy as a function of time is plotted in figure 8.6(a). We observe a generic linear increase at a shorter time



Figure 8.4: Time evolution of the two-body density  $\rho^{(2)}(x_1, x_2)$  for interaction quench  $\lambda = 15.0$ . The system relaxes to the MI state and never comes backto the initial state. All the quantities are dimensionless.

followed by saturation [Inset of figure 8.6(a)]. The sharp linear increase in Shannon information entropy S(t) is attributed to an exponential increase in the timedependent natural occupation contributing to the dynamics and is described as  $S(t) = \Gamma t \ln P$ , where  $\Gamma$  is determined by the decay probability to stay in the initial ground state and P is the number of many-body states involving in the dynamics [192]. The saturation of S(t) happens at t = 1.25 due to the complete occupation of the available finite sized Hilbert space. This is the time when the one-body density enters in the fragmented Mott insulator phase and does not come back to the initial superfluid phase. Similarly, the entropy reaches to the maximum value at time t = 1.25 never comes back to the initial phase - this makes the system to relax into the maximum entropy state.

The Shannon information entropy evolution for the lattice depth quench is shown in figure 8.6(b). It exhibits periodic oscillation. Unlike the interaction quench, the entropy  $S^{info}(t)$  for the lattice depth quench increases slowly up to



Figure 8.5: Time evolution of the two-body density  $\rho^{(2)}(x_1, x_2)$  for lattice-depth quench V = 10.1. All the quantities are dimensionless.

a maximum value then we observe a broad maxima from t = 31.0 to t = 56.0, which signifies that the system retains to its maximum entropy state which is a MI phase.  $S^{info}(t)$  goes to minimum value at t = 81.0—the same time when the many-body state revives to SF phase as depicted in figure 8.3. The collapserevival scenario same as the one- and two-body density is prominent. The absence of a generic linear increase and saturation demonstrate that the system does not relax. To check the possibility of relaxation for very strong lattice depth quench, we repeat the simulation for very deep lattice depth quench when the system is pumped with huge excitation energy. However, we do not find any signature of relaxation; the system always revives and the revival time decreases with an increase in lattice depth. But if we increase the computation time the system may eventually relax. The broad maxima of the entropy from t = 31.0 to t = 56.0in figure 8.6(b) signifies that the system retains to MI phase for this duration of time and then revives to its minimum entropy state at time t = 81.0 where SFphase is revived. Thus, t = 81.0 can be taken as the revival time for V = 10.1



Figure 8.6: (a) Time evolution of Shannon information entropy S(t) for interaction quench to  $\lambda = 15.0$ . The sharp linear increase followed by saturation signify that the system relaxes to the maximum entropy state. The inset presents the sharp linear increase fitted with the analytical formula (see text) for small time. (b) Time evolution of Shannon information entropy S(t) for lattice-depth quench V =10.1. The entropy exhibits periodic oscillation and the possibility of relaxation is ruled out. All the quantities are dimensionless.

lattice depth quench.

From the natural occupation, shown in figure 8.1(a), we know that t = 1.25 is the required time for the system to enter the MI phase and this is also the same time when the off-diagonal correlation is completely lost. The SF phase has never turned back during the long-time dynamics. The small intermediate kinks in the entropy plot in figure 8.6(a) also supports the above conclusion as the kinks never decrease up to the value corresponding to the SF phase. Thus, we can define  $t_{relax}$ in three different ways :

a) The system enters to the fully fragmented MI state for the first time.



Figure 8.7: (a) Relaxation time  $t_{relax}$  for interaction quench. The curve shows power law decay. The best fit formula is  $t_{relax} = 2.3 \ \lambda^{-0.23}$ . (b) Revival time  $t_{revival}$  for lattice-depth quench. The curve shows power law decay. The best fit formula is  $t_{revival} = 134.5 \ V^{-0.23}$ . All the quantities are dimensionless.

b) One-body diagonal correlation is only maintained.

c) The system relaxes to a steady state -maximum entropy state.

In figure 8.7(a), we plot  $t_{relax}$  for different (strong)  $\lambda$  quenches and observe a power law decay as  $t_{relax} = 2.3 \ \lambda^{-0.23}$ .

We define revival time  $(t_{revival})$  as the time when

(a) The system revives to the initial superfluid phase where the global phase coherence in one-body density is maintained.

(b) The Shannon information entropy reaches to its minimum.

In figure 8.7(b), we plot  $t_{revival}$  as a function of lattice depth which follows a power

law decay fitted as  $t_{revival} = 134.5 \ V^{-0.23}$ . The qualitative nature of variation of  $t_{revival}$  with the lattice depth resembles the same nature as observed in Greiner's experiment [45, 46]. For both interaction and lattice depth quench the system receives the same amount of excitation energy, however, the dynamical response of the system is determined by the distribution of received energy by the system. It is understandable that for interaction quench, the received energy is quickly distributed through the two-body interaction term of the Hamiltonian, thus the response time which is characterized by the relaxation time in our computation exhibits quick fall. Whereas for lattice depth quench, Hamiltonian distributes the received energy through the one-body potential, it is exhibited by the slow response of the system.



Figure 8.8: Dynamics of Shannon information entropy S(t) for small interaction quench  $\lambda = 1.0$ . The entropy shows periodic oscillation. All the quantities are dimensionless.

The dynamics for small interaction strength quench  $\lambda = 1.0$  is also discussed. Figure 8.8 reports the entropy dynamics and figure 8.9 reports the time evolution of the reduced one-body density matrix for small interaction strength quench  $\lambda=1.0$ . The amount of excitation energy received is very small, which basically induces a small perturbation to the system. The variation of entropy shows a periodic oscillation [193]. The corresponding time evolution in the one-body density matrix (figure 8.9) shows the system clearly enters in MI phase at time t = 8.5,



Figure 8.9: Time evolution of the reduced one-body density matrix  $|\rho^{(1)}(x',x)|^2$  for small interaction quench  $\lambda = 1.0$ . Collapses and revivals demonstrate how the matter-wave field dephases and rephases periodically during its time evolution. The system does not relax. All the quantities are dimensionless.

which is characterized by complete extinction of the off-diagonal correlation; however, it revives at time t = 12.5, which corresponds to the time of occurrence of first deep kink in the entropy production (figure 8.8). So we observe that only for strong interaction quench the system relaxes to steady state but for weak interaction quench, the system shows collapse-revival for long timescales. This collapse-revival dynamics is displayed in the periodic oscillation of the entropy which is in sharp contrast with generic linear increase followed by saturation for strong interaction. For completion of our work, we also present a connection between the Bose-Hubbard physics and the many-body physics in 12.1.