Chapter 6

Bose-Hubbard model with random and Fibonacci potentials

6.1 Introduction

Experimentalists are able to produce random and pseudo-random optical potentials in addition to periodic potentials by using controlled defects [128]. Recent experiments on trapped cold atoms have shown ability of loading an atomic Bose gas in a well controlled disordered potentials [46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58]. Ultra cold atoms trapped in these potentials show phases like superfluid (SF), Bose glass (BG), Mott Insulator (MI) and Density Wave (DW) [26]. It is then very interesting and exciting to study effect of quasi periodic optical potentials which are intermediate between ordered and disordered potentials. Quasi crystals have attracted a large interest since their discovery in 1984 [129]. A quasi
crystal is a long-range ordered material that does not present translational invariance, and therefore shares properties with both ordered crystals and amorphous solids [130]. Optical quasi crystal lattices have been first studied experimentally in the context of atomic laser cooling [131]. In these works, the atomic gas, which was far from quantum degeneracy, was confined in a dissipative optical lattice where coherence was lost through spontaneous emission of photons. The physics of one-dimensional quasi periodic optical lattices has been also subject of recent research in the context of cold atomic gases [132].

In this chapter we study quantum phase transitions for ultra cold bosonic atoms embedded in the random optical potential and briefly discuss the case of quasi periodic potentials.

The Bose-Hubbard model in the presence of the quasi periodic or random optical potential is given by

$$\mathcal{H} = -t \sum_{<i,j>} (a_i^\dagger a_j + h.c) + \frac{U}{2} \sum_i n_i(n_i - 1) + \sum_i \mu_i n_i. \quad (6.1)$$

For the random local potentials, $\mu_i$ is a random number distributed uniformly between $-\lambda$ and $\lambda$, i.e., $\lambda = 0$ for the pure case. As discussed in chapter 3, the Fibonacci chain is produced by using substitution rule given by, $A \rightarrow AB$ and $B \rightarrow A$. For example, if we start with $A$, first few members of the Fibonacci chain are given below. $A \rightarrow AB \rightarrow ABA \rightarrow ABAAB \rightarrow ABAABABA$. 
In the case of Fibonacci potential, $\mu_i = +\lambda$ for site $A$ and $\mu_i = -\lambda$ for site $B$. First we discussed the former case, i.e., the Bose-Hubbard model in the presence of random potential.

### 6.2 Random potential

Bose-Hubbard model in the presence of random potential has been studied by many methods [26, 27] including DMRG [67]. The main results of these studies include presence of Bose Glass phase at higher values of $\lambda$, the strength of random potential. There is no direct Mott insulator to superfluid phase transition when $\lambda$ is finite due to presence of *rare regions* in the distribution of random potentials [67, 126]. The *rare regions* are nothing but a region where the system looks pure with $\mu_i = \lambda$ or $\mu_i = -\lambda$. Below we demonstrate that even the superfluid to Bose glass transition is also governed by the presence of these *rare regions*.

First we understand the phase diagram of model (6.1) with random chemical potential based on global properties. Bosonization study of this model predict that the Luttinger Liquid parameter $K$ (defined in the chapter 2) has a value of $2/3$ at the superfluid to Bose glass transition [62, 63]. i.e., $K < 2/3$ for the superfluid phase and $K > 2/3$ for the Bose glass phase. We first reproduce these results and follow it up with analyzing the superfluid to Bose glass transition using the local compressibility as done in the chapter
The model (6.1) when $\lambda = 0$, has a superfluid to Mott insulator transition (for $\rho = 1$) with critical $U_C \sim 3.4$ (details are given in chapter 2). We now present what happens to this transition when $\lambda > 0$ analyzing (i) Luttinger liquid parameter $K$, (ii) finite size scaling of gap, i.e., $L G_L$ versus $U$ and (iii) finite size scaling of correlation length, $L / \zeta_{L}^{SF}$ versus $U$. In Figs. 6.1 and 6.2 we plot, respectively, $L / \zeta_{L}^{SF}$ and $L G_L$ versus $U$ for $\lambda = 0.4$. The coalescence of different curves corresponds to different lengths below $U < 4.0$ corresponds to a gapless phase which could be a superfluid or a Bose glass. The superfluid and Bose glass phases are identified using Luttinger Liquid parameter $K$ which is given for $\lambda = 0.4$ in Fig. 6.3 where we observe that superfluid to Bose glass phase occur at $U \sim 3.8$. The superfluid and Bose glass phases, respectively, have $K < 2/3$ and $K > 2/3$. Thus we observe that a small Bose glass phase is sandwiched between superfluid and Mott insulator phases. As $\lambda$ increases, the Bose glass phase also enlarges as demonstrated in Figs. 6.4-6.6 for $\lambda = 0.6$. Similarly the variation of $K$ keeping fixed value of $U$ and varying $\lambda$ yield the superfluid to Bose glass transition. For example Fig. 6.7 shows the variation of $K$ as a function of $\lambda$ for $U = 2$ which yield $\lambda_C \sim 3.2$ for SF to BG transition. Plots of similar type gives us the phase diagram of random Bose-Hubbard model and is given in Fig. 6.8 which in consistent with the earlier works [67]. The phase diagram is consist of SF, MI
and BG as the case discussed in the earlier chapter when the local potentials are incommensurate to the lattice.

Figure 6.1: Finite size scaling of $L/\xi_{SF}$ versus $U$ for $\lambda = 0.4$ showing gapped to gapless phase transition at $U_C \sim 4.0$. 
Figure 6.2: Finite size scaling of $LG_L$ versus $U$ for $\lambda = 0.4$ which again showing gapped to gapless phase transition at $U_C \sim 4.0$.

Figure 6.3: Variation of $K$ with respect to $U$ for $\lambda = 0.4$. The regions, respectively, below and above $K = 2/3$ is the superfluid and Bose glass
Figure 6.4: Finite size scaling of $L/\xi_{SF}^2$ versus $U$ for $\lambda = 0.6$ showing gapped to gapless phase transition at $U_C \sim 4.3$.

Figure 6.5: Finite size scaling of $LG_L$ versus $U$ for $\lambda = 0.6$ which again showing gapped to gapless phase transition at $U_C \sim 4.3$. 
Figure 6.6: Variation of $K$ with respect to $U$ for $\lambda = 0.6$. The regions, respectively, below and above $K = 2/3$ is the superfluid and Bose glass.

Figure 6.7: Variation of LL parameter $K$ with respect to $\lambda$ for $U = 2$. The regions, respectively, below and above $K = 2/3$ is the superfluid and Bose glass.
Figure 6.8: Phase diagram of model (6.1) in the presence of random local potential. There is no direct MI to SF transition and a small BG phase always intervene between them.

Though the phase diagram of model (6.1) are known, nothing much is known about the Bose glass or why there is a re-entrant, i.e., a transition from BG to SF and then back to BG for certain range of parameters. To throw more light on this we re-analyze model (6.1) using the methods described in the previous chapter, i.e., the local compressibility. We plot $\rho_i$ versus $\mu_i^{ef}$, obtained as described in the previous chapter, in Fig. 6.9 for three different realization keeping $\lambda = 0.6$ and $U = 2$. For comparison, we have also plotted the $\rho_i$ versus $\mu_i^{ef}$ curve for the pure case, i.e., for $\lambda = 0$. First thing we notice is that the general behavior of $\rho_i$ versus $\mu_i^{ef}$ is independent of a particular realization of random potential distribution. Local compressibility
decreases from that of the pure system. It is very instrumental to compare the behavior of $\rho_i$ versus $\mu_i^{\text{eff}}$ plots with incommensurate potentials and it is done in Fig. 6.10 for the case $\lambda = 0.6$, $U = 2$. As discussed in the previous chapter, the agreement between pure Bose-Hubbard model and model (6.1) with incommensurate potential keeping $Q = \frac{1 + \sqrt{5}}{2}$ suggest the validity of LDA [127]. However, LDA is not a good approximation when the local potentials vary abruptly as in the case of incommensurate potential with $Q = \frac{1 + \sqrt{5}}{2}$ or the random potentials. The most striking result is that the $\rho_i$ versus $\mu_i^{\text{eff}}$ behavior agree when the local potentials are (i) incommensurate with $Q = \frac{1 + \sqrt{5}}{2}$ and (ii) random. The compressibility, slope of $\rho_i$ versus $\mu_i^{\text{eff}}$ plot is finite everywhere and so the system is in the superfluid phase, which should be the case comparing the phase diagram Fig. 6.8.

Increasing the value of $\lambda$ we observe that the behavior of $\rho_i$ versus $\mu_i^{\text{eff}}$ plots are similar to the one discussed in the previous chapter for the incommensurate cases. For example, such plots are given in Figs. 6.10 and 6.11, respectively for $\lambda = 3$ and 5. The similarity of the behavior between different types of local potential suggest that the formation of Bose Glass phase when $U < U_C \sim 3.4$ is similar in all cases, i.e., random and incommensurate, and the Bose glass is of type BG-I. In other words, the type of inhomogeneity do not depend on the formation of Bose glass phase. This behavior of similarity in the formation of Bose glass phase continue to hold even when $U > U_C$. 
For example, we plot $p_i$ versus $\mu_i^{\text{eff}}$ curve in Fig. 6.13 for $U = 12$, $\lambda = 1$ and $\rho = 0.84$ along with that for the pure system for comparison. Again we see that the agreement between random and pure system $p_i$ versus $\mu_i^{\text{eff}}$ plot is quite good when we are away from MI region. As we approach the MI plateau, the deviation enhances. For $\lambda = 1$, the system is still in the superfluid case because the local compressibility is finite everywhere in the lattice. As we did in the case of $U < U_C$, we compare the behavior of $p_i$ as a function of $\mu_i^{\text{eff}}$ in all cases in Fig. 6.14. Plot for random, i.e., Fig. 6.14(c) agree well with that for incommensurate potential with $Q = \frac{1+\sqrt{5}}{2}$ as was the case for $U < U_C$. The formation of Bose glass, BG-II phase is again similar to that of the incommensurate potential cases. For example, Figs. 6.15 for $\lambda = 2$ where we $p_i$ versus $\mu_i^{\text{eff}}$ for all cases. The formation of plateau again suggests that the lattice breaks into superfluid and Mott insulator region. Thus a BG-II phase.
Figure 6.9: Variation of $\rho_i$ as function of $\mu_i^{eff}$ for $\lambda = 0.6$, $U = 2$ and $\rho = 1$ for three different realizations of random distribution along with that for pure system, $\lambda = 0$. 
Figure 6.10: Comparison of $\rho_i$ as function of $\mu_i^{eff}$ for $\lambda = 0.6$, $U = 2$ and $\rho = 1$. (a) and (b) for incommensurate potential with $Q = \frac{1+\sqrt{6}}{2}$ and $Q = \frac{1+\sqrt{6}}{10}$ respectively. (c) is for random and (d) is for pure, i.e., $\lambda = 0$.

Figure 6.11: Comparison of $\rho_i$ as function of $\mu_i^{eff}$ for $\lambda = 3$, $U = 2$ and $\rho = 1$. (a) and (b) for incommensurate potential with $Q = \frac{1+\sqrt{6}}{2}$ and $Q = \frac{1+\sqrt{6}}{10}$ respectively. (c) is for random and (d) is for pure, i.e., $\lambda = 0$. 
Figure 6.12: Comparison of $\rho_i$ as function of $\mu_i^{eff}$ for $\lambda = 5, U = 2$ and $\rho = 1$. (a) and (b) for incommensurate potential with $Q = \frac{1+i\sqrt{3}}{2} \text{ and } Q = \frac{1+i\sqrt{3}}{10}$ respectively. (c) is for pure, i.e., $\lambda = 0$ and (d) is for random.

The important of rare region in the MI to BG transitions have been discussed in the literature earlier [126]. We now extend these discussion for the case of SF to BG-I and BG-II transitions based on our understanding of these phases from local compressibility.

First we will discuss the SF to BG-II transition when $U > U_C$ and $\rho \neq 1$. As we discussed in detail in the previous chapter, the BG-II phase is possible (i) whenever $\mu_i^{eff}$ satisfies the condition $\mu_i^{-}(U, \lambda) < \mu_i^{eff} < \mu_i^{+}(U, \lambda)$, the local density $\rho_i$ is pinned to an integer (for example see Fig 6.15 for $U = 12, \rho = 0.84$) and (ii) the $\mu_i$ vary across the lattice smoothly. If it vary fast, the MI region get smeared out and BG-II is not possible. The rare regions
Figure 6.13: Variation of $\rho_i$ as function of $\mu_i^{\text{eff}}$ for $\lambda = 1$, $U = 12$ and $\rho = 0.84$ for three different realizations of random distribution along with that for pure system, $\lambda = 0$
Figure 6.14: Comparison of $\rho_i$ as function of $\mu_i^{\text{eff}}$ for $\lambda = 1$, $U = 12$ and $\rho = 0.84$. (a) and (b) for incommensurate potential with $Q = \frac{1+\sqrt{5}}{2}$ and $Q = \frac{1+\sqrt{5}}{10}$ respectively. (c) is for random and (d) is for pure, i.e., $\lambda = 0$.

Figure 6.15: Comparison of $\rho_i$ as function of $\mu_i^{\text{eff}}$ for $\lambda = 2$, $U = 12$ and $\rho = 0.84$. (a) and (b) for incommensurate potential with $Q = \frac{1+\sqrt{5}}{2}$ and $Q = \frac{1+\sqrt{5}}{10}$ respectively. (c) is for random and (d) is for pure, i.e., $\lambda = 0$. 
play an important role in satisfying these conditions. Since rare region acts like a pure system with a given $\mu_i = \pm \lambda$, both the conditions are easily satisfied. For example let us start from a SF region with $\rho < 1$ when $\lambda = 0$. For this system since we are starting from a SF phase, $\mu < \mu^-(U, \lambda = 0)$. Here $\mu$ is the chemical potential corresponds to the density $\rho$ defined by the Eq. (2.26). As we increase $\lambda$, spread in $\mu_i^{\text{eff}}$ increases. $\mu_i^{\text{eff}}$ can vary between $\mu - \lambda$ to $\mu + \lambda$. If we increase $\lambda$ such that $\mu_i^{\text{eff}} > \mu^-(U, \lambda)$, we get a BG-II phase. Because of the rare region this condition can easily be satisfied. Rare region can have $\mu_i = -\lambda$ such that $\mu_i^{\text{eff}} = \mu + \lambda > \mu^-(U, \lambda)$. Since the rare region acts like a pure system, there are MI region can be easily formed. This gives us critical strength of SF to BG-II transition when $\rho < 1$, given by the condition $\lambda_C = \mu^-(U, \lambda) - \mu$. Similarly for $\rho > 1$, the condition can be easily obtained and is given by $\lambda_C = \mu - \mu^-(U, \lambda)$. Since $\mu$ increases with $\rho$, $\lambda_C$ increases with increasing $(\rho - 1)$. i.e., closer the system to the MI phase, smaller the value of $\lambda_C$.

A similar arguments can be brought forward to understand the effect of rare regions in the SF to BG-I phase transition when $U < U_C$. The BG-I phase has regions with no bosons because $\mu_i$ is large enough to hold any bosons. This condition can be easily satisfied when the rare region have $\mu_i = \lambda$ and $\lambda$ is large. If the value of $\mu_i$ for a given value of $U$ which makes $\rho_i = 0$ is, say, $\mu_0(U)$, the critical value of $\lambda_C$ for the SF to BG-I transition
can be obtained in the following manner. For example if we start with a given density $\rho$, the $\lambda_C = \mu - \mu_0$ where $\mu$ is the system chemical potential. Since $\mu$ increases with $\rho$, $\lambda_C$ increases with $\rho$.

Now we re-examine the question of possibility of direct SF to MI transition in the presence of disorder. Let us start from a MI phase i.e., $U > U_C$ and $\rho = 1$. The chemical potential corresponds to this system can be obtained from the $\mu^+(U, \lambda = 0)$ and $\mu^-(U, \lambda = 0)$ and is given by $\mu = (\mu^+(U, \lambda = 0) + \mu^-(U, \lambda = 0))/2$. As we increase $\lambda$, the range of values $\mu_{i}^{\text{eff}}$ have in the lattice increases because $\mu_{i}^{\text{eff}} = \mu \pm \mu_i$. If condition $\mu^-(U, \lambda) < \mu_{i}^{\text{eff}} < \mu^+(U, \lambda)$ is satisfied for all $i$, then the system continue to be in the MI phase. As soon as some sites have $\mu_{i}^{\text{eff}} < \mu^-(U, \lambda)$ or $\mu_{i}^{\text{eff}} > \mu^+(U, \lambda)$, those sites will be in the superfluid region and the system goes over to the BG-II phase. We learned from the previous chapter that the Mott insulator region will survive when the system has inhomogeneity if the local potential vary smoothly across the lattice. The presence of rare region satisfies this condition. The disorder system can always have a rare region which has a uniform $\mu_{i}^{\text{eff}}$ such that the condition $\mu^-(U, \lambda) < \mu_{i}^{\text{eff}} < \mu^+(U, \lambda)$ is always satisfied. And these rare region will be then a Mott insulator and the rest of the system can be in the superfluid making it a BG-II phase. We can estimate an upper bound for the critical strength $\lambda$ for the MI to BG-II transition. For a disorder system, the rare regions can have $\mu_{i}^{\text{eff}} = \mu - \lambda$ so the critical
strength for MI to BG-II transition is given by $\mu^-(U, \lambda_C) = \mu - \lambda_C$. Since

$$\mu = \frac{(\mu^+(U, \lambda) + \mu^-(U, \lambda))}{2}, \lambda_C \sim \mu - \mu^-(U, \lambda) = \frac{\mu^+(U, \lambda) - \mu^-(U, \lambda)}{2} - \mu^-(U, \lambda) = \frac{G(U, \lambda)}{2},$$

where $G(U, \lambda) = \mu^+(U, \lambda) - \mu^-(U, \lambda)$ is the gap in the single particle energy spectrum. For incommensurate system as discussed in the previous chapter, for small $U - U_c$, $\mu^+(U, \lambda) \sim \mu^-(U, \lambda)$, the Mott insulator region get completely smeared out, thus $\lambda_C = 0$ giving us a direct MI to SF transition. However, this does not happen in the case of disordered system. The presence of the rare region, which acts like a pure system, always help formation of MI region and $\lambda_C$ is always finite. In other words, there is always a BG-II Phase intervene between MI and SF transition in the presence of disorder due to existence of rare regions.

And finally we re-address the re-entrant phenomena seen in the phase diagram Fig 6.8 obtained based on the global properties of the different phases. For small values of $U - U_c$, we see from the Fig 6.8 that the phase changes from BG to SF and then back to BG as we increase $\lambda$. As we discussed in the last chapter, superfluid phase appear in the inhomogeneous Bose Hubbard model for $U > U_c$ whenever the Mott insulator region is smeared out due to the presence of local chemical potential. If the variation of the local potential across the lattice is not very smooth over many lattice points, MI region is not energetically favored and if the strength of the inhomogeneous potentials is not very large, system prefers to be in the superfluid phase. This is the
reason why we get re-entrant phenomena. This scenario changes whenever there is a rare region in the system. In the presence of rare region, it can have $\mu^\text{eff}_i$ such that $\mu^-(U, \lambda) < \mu^\text{eff}_i < \mu^+(U, \lambda)$, then these rare regions will have $\rho_i = 1$ and local compressibility $\kappa_i = 0$, thus a Mott insulator phase. In other words, whenever, $U > U_C$, the possibility of rare region falls into a Mott region is high, then the system is in the BG-II phase and it is not possible to have a re-entrant to SF. The only phase transitions possible for $U > U_C$ is MI to BG-II.

In the conclusion we have discussed the phase diagram of the disordered Bose Hubbard model based on the global properties and the local compressibility. Analyzing the model from the local compressibility point of view we observed that the rare region play very important role in the phase transition from SF to BG and MI to BG phases. There can not be a direct SF to MI, and re-entrant BG-SF-BG transitions in the disorder Bose Hubbard model due to the existence of rare regions.

### 6.3 Fibonacci chain

In this section very briefly discussed the Bose Hubbard model (6.1) defined in a Fibonacci chain. As discussed in chapter 3, the Fibonacci chain is produced by using substitution rule given by, $A \rightarrow A^kB$ and $B \rightarrow A$. If $k = 1$ and 2, we get, respectively, Fibonacci chain with Golden and Silver
means. For example, if we start with A, first few members of the Fibonacci chain with Golden mean are given below. $A \rightarrow AB \rightarrow ABA \rightarrow ABAAB \rightarrow ABAABABA$. The Bose Hubbard chain with Fibonacci potential is obtained by setting $\mu_i = +\lambda$ for site A and $\mu_i = -\lambda$ for site B or vice versa. First we discussed the case $U = 2$. Since the lattice has just two values of $\mu_i$, either $\lambda$ or $-\lambda$, the $\mu_{i}^{\text{eff}}$ takes two values, $\mu - \lambda$ and $\mu + \lambda$. The corresponding $\rho_i$ can be obtained from our DMRG method and is given in Fig 6.16 for $U = 2$, $\lambda = 1$ and density $\rho = 1$ along with that for incommensurate potential with $Q = \frac{1+\sqrt{5}}{2}$. The behavior of $\rho_i$ versus $\mu_{i}^{\text{eff}}$ agree well with that of the incommensurate potential with $Q = \frac{1+\sqrt{5}}{2}$. A similar conclusion can also be drawn when $U > U_c$, say $U = 12$. For example the variation of $\rho_i$ with respect to $\mu_{i}^{\text{eff}}$ is given in Fig. 6.17. From these comparison we believe that the phase transition in the Fibonacci chain is similar to the one we obtained when the potential is incommensurate. The phases will be consist of superfluid, Mott insulator and Bose glass.
Figure 6.16: $\rho_i$ versus $\mu_{i,\text{eff}}$ for Fibonacci potential for $U = 2$, $\lambda = 1$ along with that for incommensurate potential with $Q = \frac{1+\sqrt{5}}{2}$, Golden mean.

Figure 6.17: $\rho_i$ versus $\mu_{i,\text{eff}}$ for Fibonacci potential for $U = 12$, $\lambda = 1$ along with that for incommensurate potential with $Q = \frac{1+\sqrt{5}}{2}$, Golden mean.