Chapter 4

Hard core Bosons

4.1 Introduction

In this chapter we focus our attention on the model (3.1) in the hard-core limit, i.e., taking \( U = \infty \). In this limit with density of bosons \( \rho = 1/2 \) the model (3.1) can be mapped into spin-\( \frac{1}{2} \) XX model in the presence of local magnetic field. If we include the nearest neighbor interaction term of the form \( V n_i n_j \) into the model (3.1), we get extended Bose-Hubbard model and in the hard core boson limit, it can be mapped into XXZ model in the presence of nearest neighbor interaction. In the hard core limit, every site has only two possible boson states and in the Fock state representation these states are \( |0\rangle \) and \( |1\rangle \), respectively, for states with zero and one boson. Thus the term \( \frac{U}{2} \sum_i n_i(n_i - 1) \) in the model (1.1) can be dropped because it becomes zero. In this limit, the extended Bose Hubbard model become

\[
\mathcal{H} = -t \sum_{<i,j>} (a_i^\dagger a_j + h.c) + V \sum_{<i,j>} n_i n_j + \sum_i \mu_i n_i. \quad (4.1)
\]
Since we have now only two states per site, we can map this into a spin-1/2 Hamiltonian with the identification of \( |0\rangle \equiv |\downarrow\rangle \) and \( |1\rangle \equiv |\uparrow\rangle \). Here \( |\downarrow\rangle \) and \( |\uparrow\rangle \) are, respectively, spin-\( -\frac{1}{2} \) and \( \frac{1}{2} \) states. Now using the transformations \( a_i^+ \rightarrow S_i^+ \), \( a_i \rightarrow S_i^- \), and \( \hat{n}_i \rightarrow (S_i^x - \frac{1}{2}) \), the model (4.1) maps onto the spin-\( \frac{1}{2} \) XXZ model defined as

\[
\mathcal{H}_{XXZ} = -2t \sum_{<i,j>} (S_i^x S_j^x + S_i^y S_j^y) + V \sum_{<i,j>} S_i^z S_j^z + \sum_i \mu_i S_i^z
\]

where we have the suppressed constant terms. The local chemical potential now act as a local magnetic field. In the limit of zero magnetic field, this model has been solved exactly [123, 124, 125] and shows a KT-type transition from XY to Ising ordering at \( V = 2t \). The bosonic analogs of XY and Ising phases are, respectively, SF and DW phases.

In this chapter, we first reproduce, in Sec. (4.2), all the known results of pure XXZ model using our FS-DMRG code. Our results in the presence of non-zero local chemical potential is given in the following Sections: in Sec. (4.3) commensurate potential and Sec. (4.4) incommensurate potential.

### 4.2 Pure XXZ Model

Pure XXZ model shows a KT transition from XY ordering to Ising ordering [123]. In the language of bosons this corresponds to SF to DW transition. In order to reproduce these results we calculate as described in Sec. (2.6)
1. Luttinger Liquid parameter $K$,

2. single particle gap and its finite size scaling

3. local number density and

4. DW order parameter.

Bosonization studies \[62, 63\] show that for non-interacting ($V = 0$) pure systems, Luttinger Liquid (LL) parameter $K$ is always equal to $1$, the SF and DW phases have, respectively, $K < 2$ and $K > 2$ and the transition between them is at $V_C = 2$. We verified these results in Fig. 4.1 - 4.4. In Fig. 4.1, we plot SF correlation function defined by Eq. (2.20), $\Gamma^{SF}(r)$ against $r$ and in the limit $r \to \infty$, $\Gamma^{SF}(r) \sim r^{-K/2}$ with LL parameter $K = 1 \pm 0.03$. The variation of LL parameter with interaction $V$ is given in Fig. 4.2 where we find that LL parameter $K$ increases with $V$ and $K = 2$ at $V_C = 2.0$. The DW phase has non zero gap which can be seen in Fig. 4.3 where we plot finite size scaling of gap i.e., $LG_L$ against $V$ for different system lengths $L$. The non-coalescence of different lines above $V = V_C = 2$ suggest opening of gap at $V_C = 2$ confirming SF-DW transition. Fig. 4.4 shows variation in number density $n_i$ with respect to $i$ showing density oscillation.
Figure 4.1: Correlation function $\Gamma^S_F(r)$ is plotted against $r$ for non-interacting ($V = 0$) pure system. The continuous line is the fit with $\Gamma(r)^S_F \sim r^{-K/2}$ which gives us $K = 1.0 \pm 0.03$

Figure 4.2: Variation of LL parameter $K$ with respect to $V$ which shows $K = 2$ at $V_C = 2$. 
Figure 4.3: Finite size scaling of gap $L G_L$ is plotted against $V$ for different lengths. Different curves coalesce for $V < V_C = 2$ showing SF-DW transition.

Figure 4.4: Variation of number density $\rho_i = \langle n_i \rangle$ with respect to $i$ for $V = 3$ showing DW phase. The DW oscillation dye out at the center due to the fact that the system size is even and has a left-right symmetry.
4.3 Periodic Commensurate Potential

We now extend our study for the case with non zero local chemical potential. The SF to DW phase transition discussed in the previous section get modified in the presence of finite local chemical potential $\mu_i$. We start with a simple case, i.e., $\mu_i$ is periodic and commensurate with the lattice and the last term of model 4.1 is set as,

$$\mu_i = \lambda \cos(Qi)$$

with $Q = \pi$. By varying $\lambda$ one can vary the strength of the potential.

In the presence of the commensurate potential, the competition is between $t$, $V$ and $\mu_i$. The kinetic energy encourages the bosons to form a superfluid, however, the interaction and chemical potential tend to localize the bosons destroying the superfluidity. Thus we expect to see a superfluid to non-superfluid transition either as a function of $V$ or $\lambda$.

First we study the non-interacting i.e., $V = 0$ case. In Fig. 4.5 we plot gap $G_L$ as function of $1/L$ for two different values of $\lambda = 0$ and 0.5. The single particle gap which is zero for $\lambda = 0$ opens up for any finite values of $\lambda$ suggesting a non superfluid phase when $\lambda > 0$. The variation of $G_\infty$ with respect to $\lambda$ as well as scaling of gap as given, respectively in Fig. 4.6 and Fig. 4.7 to confirm this behavior. In order to understand the nature of this non superfluid phase we have calculated the local density $\rho_i = \langle n_i \rangle$ and is
plotted in Fig. 4.8 showing a clear density wave ordering.

Figure 4.5: Gap $G_L$ is plotted against $1/L$ for $\lambda = 0.0$ and $\lambda = 0.5$.

Similar results are also obtained for finite $V$. Fig. 4.9 shows similar behavior as non-interacting case. From them, we obtain the phase diagram of model (4.1) with periodic commensurate potential and is given in Fig. 4.10. The phase diagram is consist of superfluid phase for $0 \leq V \leq 2$, $\lambda = 0$ and a density wave phase elsewhere.
Figure 4.6: Variation of $G_{\infty}$ with respect to $\lambda$.

Figure 4.7: Finite size scaling of gap $LG_L$ is plotted against $\lambda$ for $V = 0$ for different lengths. The coalescence of different curves is lost as soon as $\lambda$ is finite, which shows opening up of the single particle energy gap for $\lambda > 0$. 
Figure 4.8: Variation of number density $\rho_i$ with respect to lattice site $i$ confirming the DW phase for $V = 0$, $\lambda = 0.5$.

Figure 4.9: Finite size scaling of gap $L_{GL}$ is plotted against $\lambda$ for $V = 1.0$ for different lengths. This also shows opening up of the gap for $\lambda > 0$. 
4.4 Periodic Incommensurate Potential

We now extend our calculation for the case of periodic incommensurate potential. To produce the periodic incommensurate potential the last term of model (4.1) is set as,

$$\mu_i = \lambda \cos(Qt)$$

with $Q = \frac{1 + \sqrt{5}}{2}$, the golden mean which make it incommensurate with the lattice. In this case also, the competition is between $t$, $V$ and $\lambda$, the strength of $\mu_i$. Vidal et al. had modified the Bosonization study of Bose-Hubbard model for the case of quasi periodic potentials [122]. This study yielded using the RG flow equation, the insulating phase for fermionic system with
Luttinger Liquid parameter $K > 1$. Since the hard core limit of the model (4.1) can be mapped into spinless fermion, we believe this result hold good and use Luttinger Liquid parameter $K$ to distinguish SF ($K < 1$) and BG ($K > 1$) phase.

Our calculation of LL parameter for different values of $V$ and $\lambda$ yielded $K$ always greater than 1. This is expected because the hardcore Bose-Hubbard model at density $\rho = 1/2$ is equivalent to spinless fermion and an insulator phase results for any value of disorder [60, 61]. However, in the presence of nearest neighbor interaction, density wave phase will appear for large values of $V$.

Figure 4.11: Finite size scaling of correlation length $L/\xi^\text{SF}_L$ is plotted against $V$ for $\lambda = 0.2$ and for different lengths. Coalescence of different plots below $V < V_C = 2.0$ shows opening of gap for $V > V_C$. 
In order to obtain the phase diagram of model (4.1) with incommensurate potential, we study the finite size scaling of correlation length for different parameters, i.e., plots similar to Fig. 2.5. In the Fig. 4.11, $L/\zeta_L^{SF}$ is plotted for different lengths $L$ for $\lambda = 0.2$. The coalescence of $L/\zeta_L^{SF}$ curves of different lengths happens for $V < V_C = 2.0$ which is same as the case of $\lambda = 0$. (To calculate the critical $V$, we use the following benchmark. For pure system, i.e., $\lambda = 0$, the SF-DW transition occurs at $V_C = 2$. In other words, plots of $L/\zeta_L^{SF}$ for different values of length $L$ should coalesce for $V < V_C$. To numerically consider two curves coalesce, we obtain the value of $L/\zeta_L^{SF}$ at $V = V_C$. For example, the values of $L/\zeta_L^{SF}$ for lengths $L = 90$ and $L = 100$ is 0.1. We take this as a benchmark to decide the critical value of $V$ at which system enters from gapless to gapped phase for disordered systems. i.e., if the values of $L/\zeta_L^{SF}$ for $L = 90$ and $100$ are less than 0.1, we take the curves are coalesced and the corresponding region is gapless and if the values are greater than 0.1, the gap is finite.) Following this benchmark we obtain the $V_C(\lambda = 0.2) = 2$.

Similar plots for $\lambda = 0.6$ is given in the Fig. 4.12 and it shows that the coalescence of $L/\zeta_L^{SF}$ curves of different lengths at $V < V_C = 2.05$. The critical value for BG-DW transition increases for higher values of $\lambda$. However, Fig. 4.13 shows that LL parameter as a function of $V$ which shows $K < 2$ for $V < 2.05$ and $K > 2$ for $V > 2.05$. This suggest the critical value for
LL parameter for BG to DW transition remain as $K = 2$. This is, however, is not true for higher values of $\lambda$. The BG to DW transition do not occurs at $K = 2$. For example for $\lambda = 1.5$, $V_C = 2.5$ from finite size scaling of correlation length, $L/\zeta_L$, but the LL parameter is much larger than 2 at this point.

The Fig. 4.14 shows the coalescence of $L/\zeta_L^{SF}$ curves of different lengths at $V_C = 2.1$ and Fig. 4.15 shows that LL parameter $K = 2$ at the same point. The $V_C$ is increasing further as $\lambda$ increases. The trend becomes more clear when $\lambda$ is increased further. The Fig. 4.16 shows opening of gap at $V_C = 2.5$. But in this case LL parameter $K = 2$ is at $V = 2.25$.

DW phase is also confirmed by Fig. 4.18 where number density $\rho_i$ is plotted against $i$ for $\lambda = 1.0$. We see density oscillations for $V = 3.6$ and no such oscillations for $V = 1.0$. These density oscillations confirm DW phase. Fig. 4.19 shows the plot of DW order parameter against $1/L$ for $\lambda = 0.6$ varying $V$ from 1.0 to 4.6 at the step of 0.2. Extrapolating $O_{DW}$ to $L \to \infty$ yield finite DW parameter for $V > V_C \sim 2$.

Plots of these kinds as well as the keeping $V$ fixed and varying $\lambda$, for example Fig. 4.20 for $LG_L$ versus $\lambda$, we obtain the phase diagram of periodic incommensurate case in hard core limit of model (4.1) and is given in Fig. 4.21. For $0 \leq V \leq 2.0$ and $\lambda = 0$ SF phase is observed. For finite values of $\lambda$, BG phase exist and for higher values of $V$ there exist a phase transition
from BG to DW. The critical value of \( V_C \) for this transition increases with increase in \( \lambda \).

We now conclude this chapter by highlighting our main results. In this chapter we study the extended Bose-Hubbard model in the hard core limit. First we reproduced all the known results of the model (4.1) in the absence of any additional potential. In this limit, we observe the known superfluid to density wave transition as we increase the nearest neighbor interaction \( V \) with a critical value \( V_C = 2 \). In the presence of either periodic commensurate or incommensurate potential, the model (4.1) does not support a superfluid phase for non-zero \( \lambda \). In the case of commensurate potential, the density wave stabilizes as soon as \( \lambda \) is finite. However, in the case of incommensurate potential, Bose glass phase is more stable than density wave for small values of \( V \), however, density wave is stable for higher values of \( V \). Value of \( V_C \) for BG-DW transition increases as \( \lambda \) i.e. disorder strength increases. For a smaller values of \( \lambda \), \( V_C \) at which gap opens up and value of \( V \) at which LL parameter \( K \) becomes 2 coincides. But as \( \lambda \) increases these values differ from each other.
Figure 4.12: $L/\zeta^{SF}$ is plotted against $V$ for different lengths keeping $\lambda = 0.6$.

Figure 4.13: Plot of LL parameter $K$ versus $V$ for $\lambda = 0.6$ which shows $K = 2$ at $V_G = 2.05$. 
Figure 4.14: $L/\zeta_{\text{SF}}^L$ is plotted against $V$ for $\lambda = 0.8$, for different lengths showing opening of gap at $V_C = 2.1$.

Figure 4.15: Plot of LL parameter $K$ versus $V$ for $\lambda = 0.8$ which shows $K = 2$ at $V_C = 2.1$. 
Figure 4.16: $L/\zeta_L^{SF}$ is plotted against $V$ for $\lambda = 1.5$, for different lengths. This shows opening of gap at $V_C = 2.5$.

Figure 4.17: Plot of LL parameter $K$ versus $V$ for $\lambda = 0.8$ which shows $K = 2$ at $V_C = 2.25$. 

Figure 4.18: Variation of number density $\rho_i$ with respect to lattice site $i$ for $V = 1.0$ and $V = 3.6$ which confirms DW phase for $V = 3.6$. The DW oscillation dye out at the center due to the fact that the system size is even and has a left-right symmetry.

Figure 4.19: DW order parameter is plotted against $1/L$ for $\lambda = 0.6$. $V$ vary from below to above between 1.0 to 4.6 at the step of 0.2.
Figure 4.20: Finite size scaling of gap $L_{G_L}$ is plotted against $\lambda$ for $V = 4.0$ for different lengths. This shows opening up of the gap for $\lambda < 3.0$.

Figure 4.21: Phase diagram of model (4.1) when periodic incommensurate potential is finite in the hard core limit.