Quantum Phase Analysis of Extended Bose-Hubbard Model

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We have obtained the quantum phase diagram of one dimensional extended Bose-Hubbard model using the density-matrix renormalization group and Abelian bosonization methods for different commensurabilities. We describe the nature of different quantum phases at the charge degeneracy point. We find a direct phase transition from Mott insulating phase to superconducting phase for integer band fillings of bosons. We predict explicitly the presence of two kinds of repulsive Luttinger liquid phases, apart from the charge density wave and superconducting phases for half-integer band fillings. Our study reveals that extended range interactions are necessary to get the correct phase boundary of an one-dimensional interacting bosons system.

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1. INTRODUCTION

We present the quantum phase diagram (QPD) of extended Bose-Hubbard model (EBH) \textsuperscript{1,2,3}, for spinless bosons on a one-dimensional lattice. These bosons could represent Cooper pairs undergoing Josephson tunneling between superconducting islands or Helium atoms moving on a substrate. Here we are interested in the quantum phase transitions of the ground state. This transition is driven by quantum fluctuations of the system which are controlled by the system parameters \textsuperscript{1,2}. There are a few experiments carried out on one-dimensional Josephson junction systems of different lengths under a magnetic field \textsuperscript{2,3,4,5,6,7,8}; a superconductor-Mott insulator transition is observed. In these systems, relevant particles are the Cooper pairs which can be treated as spinless charge bosons. Hence the Bose-Hubbard model and its variants are prominent candidates to study such systems. It is also revealed from experiments that the inter-particle interactions are of finite range \textsuperscript{2,3,4,5,6,7,8}. We study an EBH model that incorporates the nearest-neighbor (NN) and next-nearest-neighbor (NNN) repulsive interactions in addition to the on-site Hubbard repulsion. We also consider the NN and NNN hopping of bosons on the lattice. In what follows, we derive an analytical expression for Mott insulating gap at the mean-field limit but this alone is not sufficient to capture the effects of all interactions especially at the charge degeneracy point \textsuperscript{9}. We map our EBH model to a spin chain model, for strong on-site Coulomb repulsions. In this letter, we first present the results of Abelian bosonization study of spin chain model, we then discuss the results of our Density Matrix Renormalization Group method (DMRG) \textsuperscript{10} study of the EBH model.

The model Hamiltonian representing, arrays of superconducting (SC) nano-island, here after referred to as superconducting quantum dots (SQD) is given by,

\[ H = -t_1 \sum_i (\hat{b}_i^\dagger \hat{b}_{i+1} + h.c) - t_2 \sum_i (\hat{b}_i^\dagger \hat{b}_{i+2} + h.c) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + V_1 \sum_i \hat{n}_i \hat{n}_{i+1} + V_2 \sum_i \hat{n}_i \hat{n}_{i+2} - \mu \sum_i \hat{n}_i \] (1)

in the usual notation.

2. MODEL HAMILTONIANS AND CONTINUUM FIELD THEORETICAL STUDY:

We recast our basic Hamiltonians in the spin language \textsuperscript{11} to obtain; \[ H_{J1} = -2 E_{J1} \sum_i (S_i^+ S_{i+1}^- + h.c), \quad H_{J2} = -2 E_{J2} \sum_i (S_i^+ S_{i+2}^- + h.c), \quad H_{Ec0} = \frac{E_{Ec0}}{2} \sum_i (2S_i^Z - 1)^2, \]
\[ H_{Ec1} = 4E_{Z1} \sum_i S_i^+ S_{i+1}^- S_i^- S_{i+2}^+, \quad H_{Ec2} = 4E_{Z2} \sum_i S_i^+ S_{i+2}^- S_i^- S_{i+1}^+ \] Our total Hamiltonian is,

\[ H = H_{J1} + H_{J2} + H_{Ec0} + H_{Ec1} + H_{Ec2} \] (2)

Here \[ h = (N - 2n - 1)/2 \] and \textit{N} tunes the system to a degeneracy point by means a gate voltage \( eN \sim V_g \) where \( eN \) is the average dot charge induced by the gate voltage. The phase diagram is periodic in \textit{N} with period 2. Here we only consider a single slab of the phase diagram, \( 0 \leq N \leq 2 \). Correspondence between the parameters of the EBH model and the spin chain model is; \( \langle n \rangle t_1 \sim E_{J1}, \quad \langle n \rangle t_2 \sim E_{J2}, \quad U \sim E_{Ec0}, \quad V_1 \sim E_{c1}, \quad V_2 \sim E_{z2} \) \textsuperscript{12}. When the ratio \( \frac{E_{Ec0}}{E_{Ec0}} \to 0 \), the SQD array is in the insulating state with gap \( \sim E_{Ec0} \), it costs an energy \( \sim E_{Ec0} \) to increase by one, the number of pairs on a given dot. Exceptions are the discrete points at \( N = 2n + 1 \), where a dot with charge \( 2ne \) or \( 2(n + 1)e \) has the same energy because gate charge compensates the charges of extra Cooper pair in the dot. At this degeneracy point, a small amount of Josephson coupling leads the system to the SC state. To analyze the phases explicitly near this
degeneracy point, we recast the Hamiltonian of the spin chain model to a spinless fermion model through Jordan-Wigner transformations and carry out a continuum field theoretical study of spinless fermion model [13]. Our continuum models, in terms of bosonic fields [14], are

\[ H_1 = H_0 - \frac{4E_{Z1}}{(2\pi \alpha)^2} \int \cos(4\sqrt{K} \phi(x)) \, dx + \frac{2\hbar E_{C0}}{\pi} \int \partial_x \phi \, dx. \]  

(3)

\[ H_2 = H_0 - \frac{4E_{Z2}}{(2\pi \alpha)^2} \int \cos(4\sqrt{K} \phi(x)) \, dx + \frac{2\hbar E_{C0}}{\pi} \int \partial_x \phi \, dx. \]  

(4)

\[ H_0 = \frac{v}{\pi} \int dx \left[ (\partial_x \theta)^2 + (\partial_x \phi)^2 \right], \]  

is the non-interacting part of the Hamiltonian (Eq.2). The velocity, \( v \), of low energy excitations is one of the Luttinger liquid (LL) parameters while \( K \) (Eqs. 3 and 4) is the other.

\( \phi \) field corresponds to the quantum fluctuations (bosonic) of spin and \( \theta \) is the dual of \( \phi \). They are related by \( \phi_R = \theta - \phi \) and \( \phi_L = \theta + \phi \). The effect of applied gate voltage on the SQD appears as an effective magnetic field in the spin representation of these Hamiltonians. In \( H_1 \), we consider the NN Josephson coupling, on-site and NN charging energies of SQD and also the NN charging energy correction for the co-tunneling process. In \( H_2 \), we consider all the interactions present in our Hamiltonian besides all terms of co-tunneling process [11, 14]. Analytical expressions for \( E_{Z1} \) and \( E_{Z2} \) are \( E_{Z1} = \frac{4E_{J1}^2}{16E_{C0}} \) and \( E_{Z2} = \frac{3E_{J2}^2}{16E_{C0}} - \frac{3}{2}E_{Z2} \) respectively.

3. NUMERICAL STUDIES

We use the DMRG method to numerically study the QPD of the Hamiltonian in Eq. 1. We employ the infinite DMRG algorithm keeping 128 density matrix eigenvectors. The site boson Fock space is truncated to three and the number of sites in the chain is restricted to 128. Per site bosonic filling fractions 0.5 and 1.0 are studied. Accuracy of the method is checked by comparing the ground state energies, various correlation function and charge gap from DMRG studies with exact diagonalization studies of small systems. We have also reproduced the result of earlier DMRG calculations satisfactorily [3]. The discarded density in the DMRG calculations is less than \( 10^{-14} \) in the charge density wave (CDW) phase at \( \rho = 0.5 \) as well as in the Mott-insulating phase at \( \rho = 1.0 \). However, the discarded density is slightly less than \( 10^{-10} \) in the SC phase. For calculating the correlation function, we target only the ground state. To obtain the Berezinskii-Kosterlitz-Thouless (BKT) transition point, we plot the correlation function \( \langle b_x^c b_0 \rangle \) vs \( r \) on a log-log plot, here \( r = 0 \) is the middle site in the chain. The slope of this plot in the region between \( r = 16 \) and \( r = 36 \) gives \(-K/2\), where \( K \) is the Luttinger liquid (LL) parameter (Eqs. 3 and 4). The BKT-point corresponds to slope of -1 for \( \rho = 0.5 \) and -0.25 for \( \rho = 1.0 \).

4. PHYSICAL ANALYSIS OF QPDS.

Here we analyze the QPD of Hamiltonian \( H_1 \) (Eq. 3). The analytical structure of this model is the same as that of the XXZ Heisenberg chain in a magnetic field. Hence, LL parameter of \( H_1 \) can be calculated exactly by using the Bethe-ansatz techniques. Analytical expression for \( K \) [12] is of the form

\[ K = \frac{\pi}{\pi + 2 \sin^{-1} \Delta}, \]  

(5)

where \( \Delta \) is the XXZ anisotropy parameter of the Heisenberg chain. Our analysis will use the two limits of the parameters \( \Delta \), namely \( \Delta_1 \) and \( \Delta_2 \); the analytical expressions for these are \( \frac{2E_{Z1}}{E_{J1}} \) and \( \frac{2E_{Z1} - 3E_{J2}}{E_{C0}} \) respectively.

We calculate the analytical expression for the LL parameter for Hamiltonian \( H_2 \) (Eq. 4) as

\[ K = \sqrt{\frac{E_{J1} - \frac{2E_{J2}E_{Z2}}{E_{J1} + \frac{2}{\pi}(4E_{Z1} - \frac{3E_{J2}}{E_{C0}})}}{E_{J1} + \frac{2}{\pi}(4E_{Z1} - \frac{3E_{J2}}{E_{C0}})}}. \]  

(6)

In the limit \( \Delta = \Delta_1 \), for \( E_{J1} < 2E_{Z1} \) and relatively small field, the anti-ferromagnetic Ising interaction dominates
FIG. 2: Phase diagram of $1/\xi$ vs. $t_1$ for (a) $\rho = 0.5$ and (b) $\rho = 1.0$ boson density for different values of $V_2$ ($\xi^2 = \sum_i \sum_j \langle b_i^\dagger b_j \rangle / \sum_i \langle b_i^\dagger b_i \rangle$). We predict three quantum phases: CDW, RL2 and SC phase for $\rho = 0.5$ but there is no evidence of RL2 phase for $\rho = 1.0$. Inset in (a) show structure factors for $\rho = 0.5$.

FIG. 3: Phase diagram in $(t_1, 1/\xi)$ plane for boson density of 0.5. We predict effect of finite value of $t_2$ on two phase boundaries (CDW-RL2, RL2-SC).

FIG. 4: Density-density correlation function for two values of $V_2$ at $V_1 = 0.4$. $\circ - \circ$ $t_1 = 0.05$, $\square - \square$ $t_1 = 0.1$ and $\Diamond - \Diamond$ $t_1 = 0.15$. Phases is entirely new.

In Fig. 2 we present the DMRG study of EBH model (Eq. 1) for boson densities, $\rho$, of 0.5 (Fig. 2a) and 1.0 (Fig. 2b). We predict three quantum phases, CDW, RL2 and SC for $\rho = 0.5$. There is no evidences of LL phase for integer boson density. So our field theoretical analysis is consistent with DMRG studies. The structure factor in inset of Fig. 2a for $\rho = 0.5$ precludes CDW phase for this parameter range. There is also no evidence for RL1 phase; one obtains the RL1 phase for higher values of $\mu$ (gate voltage) in the CDW regime. We observe that the boundary between CDW and RL2 phases as well as RL2-SC phase boundary shift slightly for higher values of $V_2$. Fig. 3 shows the effect of NNN hopping on the phase diagram of Fig. 2. We note that the RL2 phase and CDW region are squeezed on introducing the NNN hopping while expanding the region of SC phase. In Figs. 2 and 3 we have presented the explicit parameter dependence of QPD which is not possible to obtain from the Abelian bosonization study.

If we consider only the interaction terms of the Hamiltonian $H_1$, for both $\Delta_1$ and $\Delta_2$ limits we get the condition $E_{Z1} \leq -\frac{E_1}{4}$ for the boundary between RL1 and CDW. This condition is unphysical; we know experimentally that $E_{J11}$, $E_{J12}$, $E_{Z1}$ and $E_{Z2}$ are all positive [8, 12]. So the interaction part of Hamiltonian $H_1$ alone is not sufficient to produce the whole phase diagram of Fig. 4. It indicates that an extended interaction term is required to get the correct phase diagram. We focus phase boundary between RL2 and SC phase of $H_1$ for $\Delta = \Delta_1$ and $\Delta = \Delta_2$, similar analysis of LL parameter gives the condition $E_{Z1} < 0$ which is again unphysical. This phase boundary also requires NNN hopping and NNN coulomb interactions.

Here we do the analysis of the Hamiltonian $H_2$, which extends the range of hopping as well interactions of...
and CDW phase indicates that parameters for which RL1 and CDW phase boundary can exist. Therefore, we can find physical values of these parameters for which RL1 and CDW phase boundary can exist. Similar analysis for the phase boundary between RL2 and SC phase indicates that $H_2$ can also support such a phase boundary. $B_2$ phase of Fig. 1 can be obtained only from the analysis of Hamiltonian $H_2$ when $E_{z2}$ exceeds some critical value like in the Majumdar-Ghosh model $[15]$. The above analysis is new and a consequence of extending the range of hopping and interactions. In Fig. 1 we find two multi-critical point, $P_1$, and $P_2$. Mott, RL1, RL2, and superconducting phases coincide at the point $P_1$; RL1, RL2, and $B_1$ or $B_2$ coincide at the $P_2$ point. In our QPD, we obtained multi-critical points not only for the presence of different kinds of interactions in the SQD but also on application of external gate voltage on the SQD. In our QPD, the class of transition is changing as one moves away from the tip of the lobe in the Fig. 1. Our analysis allows to extend the classification of two types of Mott transition in the context of SQD. At the tip of each lobe, the system at fixed density is driven from the SC phase to insulating phase by changing the interaction parameter and this is Mott-U (Berezinskii-Kosterlitz-Thouless) transition. Away from the tip of the lobe, a change in the gate voltage drives the system from a SC phase to an insulating phase and this is the Mott-$\delta$ transition.

Fig. [1] shows that density-density correlation function $F(j) = \langle n_m n_j - n_j n_m \rangle$ from the middle site of the chain, $m$. We study $F(j)$ for different values of $V_2$ and $t_2$. We observe that as $V_2$ increases the system crosses over from the $2K_F$ CDW state to $4K_F$ CDW state. Increasing $t_2$ leads to decrease in CDW amplitude. The prediction of $4K_F$ CDW state is entirely new for this Hamiltonian.

In Fig. [3] we present the DMRG analysis of BKT transition for $\rho = 0.5$ and $\rho = 1.0$ for different values of $V_1$. We observe that for $\rho = 0.5$, SC phase occurs for small values of $t_1$ compared to $\rho = 1.0$. For $\rho = 0.5$, CDW phase and RL2 boundary appears at $t_1 = 0.11 \pm 0.03$ for $V_1 = 0.3$ and 0.4 for different values of $V_2$. We also note that $t_2 = 0.1$ shifts the MI-SC boundary to a much smaller value of $t_1(< 0.03)$.

In summary, we have presented the phase diagram of EBH model. Description of repulsive luttinger liquid phase regions and the $4K_F$ CDW states for higher values of $V_2$ is entirely new.

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