Competition between the Haldane insulator, superfluid and supersolid phases in the one-dimensional Bosonic Hubbard Model

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Abstract. We use quantum Monte Carlo (QMC), density matrix renormalization group (DMRG) and time evolution block decimation (TEBD) to study the competition between several exotic quantum phases in the one-dimensional extended bosonic Hubbard model and map its phase diagram. Of particular interest is the Haldane insulating phase which we show to be present only for density $\rho = 1$. We also show that the supersolid phase is present for a wide range of parameters including commensurate densities.

1. Introduction

The bosonic Hubbard model [1] has attracted enormous attention and has been exploited to understand many physical phenomena such as adsorption of bosonic atoms on surfaces[2], the effect of disorder on superfluids and the appearance of the compressible Bose glass phase [1, 3], localization of flux lines and superconducting vortices[4], universal conductivity in thin disordered films[5, 6, 7] and quantum phase transitions between strongly correlated exotic phases. In addition, in the hardcore limit, the BHM can be mapped onto Heisenberg spin models and thus offers the opportunity to study magnetic phenomena under various conditions. Study of the BHM intensified with the experimental realization of Bose-Einstein condensates and the ability to load them in optical lattices [8]. Under experimentally realizable conditions, these systems are described by the BHM and its extensions [9] with highly tunable parameters and in one, two and three dimensions.
In its simplest form, which has only on-site contact interactions, the ground state of the BHM exhibits two phases [1]. At integer filling and strong repulsion, the particles cannot hop between sites and the system is an incompressible Mott insulator (MI) which is replaced by a superfluid (SF) phase at weak coupling. At incommensurate fillings, the system is always SF. Extending this model with the addition of longer range interactions or anisotropic hopping terms leads to new exotic phases. For example, extensive quantum Monte Carlo (QMC) simulations have shown that a strong enough near neighbor repulsion can lead to insulating incompressible density wave order (CDW) at integer and half odd integer fillings. Doping these phases can lead to phase separation or to supersolid (SS) phases [10, 11, 12, 13, 14, 15, 16, 17].

At a density \( \rho = 1 \) and large contact repulsion, the BHM is in the MI phase. Quantum fluctuations in this phase allow bosons to jump to neighboring sites giving occasional vacant sites and multiply occupied sites. If one assumes that at most doubly occupied sites are present, then the system exhibits empty, singly and doubly occupied sites and can be mapped onto the \( S_z = 0, \pm 1 \) states of a spin-1 Heisenberg system. Exploiting this mapping, it was in fact shown [18, 19] that this model (with near and next near neighbor interactions) has a Haldane insulating (HI) phase [20, 21] which is a gapped phase characterized by a non-local (string) order parameter. The phase diagram at \( \rho = 1 \) was also mapped [22]. However, several important questions remain open. Does the HI exist for other integer fillings of the system or is it a special property of the unit filling case? The SS phase found in one dimension [15] was obtained by doping a CDW phase: Does this phase also exist for commensurate fillings in one dimension for parameter choices similar to those in two [23] and three dimensions [24]? If the SS phase exists for commensurate fillings, where is it situated in the phase diagram relative to the CDW, MI and HI phases? Here, we use DMRG (from the ALPS library[25]), QMC and TEBD to answer these questions. The QMC is done with periodic boundary conditions and thus allows us to sample different winding number sectors and therefore to calculate the superfluid density (see below). DMRG and TEBD calculations are performed with open boundary conditions which allows us to gauge the finite size effects compared to QMC. In addition, it is much easier to measure excited state energies and excitation spectra using DMRG and TEBD than QMC. All calculations reported here were done in the canonical ensemble.

2. The Model

The one dimensional extended BHM we shall study is described by the Hamiltonian,

\[
H = -t \sum_i (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) + \frac{U}{2} \sum_i n_i (n_i - 1) + V \sum_i n_i n_{i+1}.
\]

(1)

The sum over \( i \) extends over the \( L \) sites of the lattice, periodic boundary conditions were used in the QMC and open conditions with the DMRG and TEBD. The hopping parameter, \( t \), is put equal to unity and sets the energy scale, \( a_i \) (\( a_i^\dagger \)) destroys (creates) a boson on site \( i \), \( n_i = a_i^\dagger a_i \) is the number operator on site \( i \), \( U \) and \( V \) are the onsite and near neighbor interaction parameters.

Several quantities are needed to characterize the phase diagram. The superfluid density is given by [26]

\[
\rho_s = \frac{\langle W^2 \rangle}{2td\beta L^d - 2},
\]

(2)

where \( W \) is the winding number of the boson world lines, \( d \) is the dimensionality and \( \beta \) the inverse temperature. The CDW order parameter, \( S(k = \pi) \), the one-particle Green function and the momentum distribution, \( n_k \), are given by

\[
S(k) = \frac{1}{L} \sum_{r=0}^{L-1} e^{ikr} \langle n_0 n_r \rangle, \quad G(r) = \langle a_0^\dagger a_{r} \rangle, \quad n_k = \frac{1}{L} \sum_{r=0}^{L-1} e^{ikr} G(r).
\]

(3)
which are important to characterize the HI are the string (O)
are summarized in Table 1, where defining δn
DMRG by targeting the lowest excitation with the same number of bosons. The various phases
n particles and is obtained both with QMC and DMRG. The neutral gap, ∆
where
The charge gap is given by,

\[
\Delta_c(n) = \mu(n) - \mu(n-1) = E_0(n+1) + E_0(n-1) - 2E_0(n),
\]

where \(\mu(n) = E_0(n+1) - E_0(n)\) and \(E_0(n)\) is the ground state energy of the system with \(n\) particles and is obtained both with QMC and DMRG. The neutral gap, \(\Delta_n\), is obtained using DMRG by targeting the lowest excitation with the same number of bosons. The various phases are summarized in Table 1 where, defining \(\delta n_j = n_j - \rho\), the two non-local order parameters which are important to characterize the HI are the string \((\mathcal{O}_s)\) and parity \((\mathcal{O}_p)\) order parameters,

\[
\mathcal{O}_s(|i - j| \to \infty) = \langle \delta n_i e^{i\pi \sum_{k=1}^j \delta n_k} \delta n_j \rangle, \quad \mathcal{O}_p(|i - j| \to \infty) = \langle e^{i\pi \sum_{k=1}^j \delta n_k} \rangle. \tag{5}
\]

### Table 1. Order parameters characterizing various phases.

| \(\rho_s\) | \(S(\pi)\) | \(\Delta_c\) | \(\Delta_n\) | \(\mathcal{O}_p(L_{\text{max}})\) | \(\mathcal{O}_s(L_{\text{max}})\) |
|----------|----------|------------|------------|----------------|----------------|
| MI       | 0        | 0          | \(\neq 0\) | \(= \Delta_c\) | \(\neq 0\) |
| CDW      | 0        | \(\neq 0\) | \(\neq 0\) | \(\neq 0\) | \(\neq 0\) |
| SF       | \(\neq 0\) | 0          | 0          | 0              | 0              |
| HI       | 0        | 0          | \(\neq 0\) | \(\neq 0\) | \(\neq 0\) |
| SS       | \(\neq 0\) | \(\neq 0\) | 0          | \(\neq 0\) | \(\neq 0\) |

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where \(\mu(n) = E_0(n+1) - E_0(n)\) and \(E_0(n)\) is the ground state energy of the system with \(n\) particles and is obtained both with QMC and DMRG. The neutral gap, \(\Delta_n\), is obtained using DMRG by targeting the lowest excitation with the same number of bosons. The various phases are summarized in Table 1 where, defining \(\delta n_j = n_j - \rho\), the two non-local order parameters which are important to characterize the HI are the string \((\mathcal{O}_s)\) and parity \((\mathcal{O}_p)\) order parameters,

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\]

### 3. Results

We calculated the order parameters for a wide range of parameters using the Stochastic Green Function (SGF) QMC algorithm [27], DMRG and TEBD. To characterize the phases and map out the phase diagram, some parameters are fixed while others are varied. For example, in Fig.1 we fix \(V/U = 3/4\) and \(\rho = 1\) and calculate several physical quantities as \(t/U\) is varied. In the right panel, we show (a) the CDW \(S(k = \pi)\) and superfluid \((\rho_s)\) order parameters, (b) the string \((\mathcal{O}_s)\) and parity \((\mathcal{O}_p)\) order parameters and (c) the neutral \((\Delta_n)\) and charge \((\Delta_c)\) gaps. \(S(\pi)\) vanishes at \(t/U \approx 0.22\) beyond which \(\rho_s\) appears to be nonvanishing. However, finite size studies show that \(\rho_s \to 0\) as \(L \to \infty\) indicating that the zone \(0.22 < t/U < 0.4\) is not superfluid. At the same time, \(\mathcal{O}_s(t/U > 0.22) \neq 0\) and the gaps are nonvanishing too. This indicates that the transition at \(t/U = 0.22\) is from the CDW phase to the gapped Haldane insulating phase. As \(t/U\) increases further (not shown) the system will leave the HI and enter the SF phase. Note that in the \(\rho = 1\) CDW phase \(\Delta_c > \Delta_n\) and that \(\Delta_n\) vanishes at the CDW-HI transition but \(\Delta_c\) remains nonzero. The meaning of the two unequal gaps can be seen in the center and right panels of Fig.1 showing the dispersion, \(\omega(k)\). The charge gap is given by \(\Delta_c = \omega(k \to 0)\) while \(\Delta_n\) is the smallest excitation gap at any \(k\). The smallest gap here is at \(k = \pi\) thus giving the neutral gap \(\Delta_n = \omega(k = \pi)\). So, it is possible for \(\Delta_c\) and \(\Delta_n\) to be unequal and for one of them to vanish but not the other. At the CDW-HI \(\Delta_n\) vanishes due to the loss of order at the ordering vector \(k^* = \pi\).

The question of what happens at other fillings, especially commensurate ones, is very interesting. For example, does the HI appear at other integer fillings? We address this question in Fig.2 where we show in the left panel the same quantities as in Fig.1. These two figures exhibit some marked differences. The QMC results, Fig.2(a), show that \(\rho_s\) becomes nonzero before \(S(\pi)\) vanishes indicating the simultaneous presence of long range density order (CDW)
Figure 1. Left: Order parameters (a,b) and gaps (c) versus $t/U$ at fixed $V/U = 3/4$. Center: excitation spectrum, $\omega(k)$ at $t/U = 0.2$ (CDW). Right: excitation spectrum, $\omega(k)$ at $t/U = 0.22$ (CDW-HI transition). All are at fixed $\rho = 1$.

Figure 2. Left: Order parameters (a,b) and gaps (c) versus $t/U$ at fixed $V/U = 3/4$. Center: $G(r)$ in for $t/U = 0.325, 0.4, 0.44$. Right: excitation spectrum, $\omega(k)$ at $t/U = 0.38$, in the SS phase. All are at fixed $\rho = 2$.

and superfluidity. This is confirmed by DMRG in panel (c) which shows $\Delta_n = \Delta_c$ vanish together at $t/U = 0.37$ while the CDW order is still finite. Therefore, this region of coexistence, $0.37 < t/U < 0.425$, corresponds to the supersolid (SS) phase: No HI is apparent at $\rho = 2$. The center panel of Fig.2 shows that the one-body Green function decays as a power, $G(r) \propto r^{-1/2K}$, in the SS and SF phases, which resolves the disagreement between various bozonization results concerning the SS phase. We found $K = 2.24$ for $t/U = 0.4$ (SS) and $K = 2.5$ for $t/U = 0.44$ (SF). In the CDW phase, $G(r)$ decays exponentially. The right panel of Fig.2 shows the excitation spectrum in the SS phase. Note that $\Delta_c = \omega(k \to 0) \to 0$, indicating gapless excitations. The same is seen at $k = \pi$; in this phase $\Delta_c = \Delta_n = 0$.

By repeating such measurements at many fillings, we map out the phase diagram in the $(\mu/U, t/U)$ plane at fixed $V/U = 3/4$ and confirm the absence of the HI at all fillings except $\rho = 1$. Figure 3 shows that the $\rho = 1/2$ CDW lobe is almost entirely surrounded by SF, all lobes at $\rho > 3/2$ are surrounded by SS and the region of the $\rho = 1$ lobe which sticks out of the SS is the HI phase. The transition from the $\rho = 3/2$ CDW lobe goes directly to the SF phase without passing through SS. We verified that this behavior persists at other values of the ratio $V/U$. It is interesting to note that the HI phase is present only at $\rho = 1$ and that the SS phase is present over a large region in the phase diagram. It is particularly interesting that the SS phase exists at commensurate fillings.
Figure 3. The phase diagram at fixed ratio $V/U = 3/4$. The inset is a zoom on the tip of the $\rho = 1$ lobe. All symbols represent results from QMC simulations for $L = 128$ (stars) and $L = 64$ (all other symbols). The solid black lines near the lobe tips are DMRG results with $L = 192$. The end points of the lobes are obtained by studying the finite size dependence of $\Delta_n$ using DMRG except for $\rho = 1$ which is obtained using QMC by extrapolating $O_s$ to the thermodynamic limit.

Another informative view is to show the phase diagram at fixed density. This is given in the left panel of Fig.4. The open squares are the results of Ref. [22], all other symbols are results of our QMC simulations. Our results confirm those of Ref. [22] where the error bars are small and improve them where the error bars are large and we have determined part of the SF-HI boundary. The straight line, $U = 4V/3$, shows where the measurements leading to Fig.1 were taken. The star on this line is the tip of the $\rho = 1$ lobe in Fig.3. In addition, we have determined the boundary of a phase separation (PS) region whose presence had not been suspected in the literature. Identifying this PS is accomplished by examining the density profiles. The right panel of Fig.4 shows such a profile exhibiting an island of SS region in a sea of SF.

In Fig.3 we showed that, for $V/U = 3/4$, the HI appears only at $\rho = 1$. To explore if the HI can appear for other ratios, we map in Fig.5 the phase diagram in the $(U, V)$ plane for $\rho = 3$. This figure shares some general features with Fig.4 but there are important differences: (a) No HI phase appears anywhere in the phase diagram but instead (b) a supersolid phase appears at the tip of the CDW region.

Figure 4. Left: The phase diagram in the $(U, V)$ plane for $\rho = 1$. Right: The density profile displaying phase separation.

Figure 5. Applying the same methods as for $\rho = 1$, the $\rho = 3$ phase diagram is mapped out. Unlike for $\rho = 1$, there is no HI here but there is SS in addition to the MI, SF, CDW and PS regions.
4. Conclusions
We used QMC simulations and DMRG/TEBD calculations to determine the phase diagram of the extended bosonic Hubbard model in one dimension. Of special interest is the HI phase and where it appears in the phase diagram. The HI is a gapped insulating phase characterized by a nonlocal order parameter; it is expected to appear in the Heisenberg spin model for odd integer values of the spin. Deep in the MI lobes, one can map the BHM onto the Heisenberg model with $S = \rho$ and might then expect the HI to appear for odd values of $\rho$. We have determined the phase diagram in the $\mu/U$, $t/U$ plane for $V/U = 3/4$ and confirmed that the HI is indeed present for $\rho = 1$ but we found that it is absent at all other densities. This absence is again confirmed by mapping the $\rho = 3$ phase diagram in the $(U, V)$ plane where it is shown that a SS phase appears but no HI. Furthermore, we showed that the phase diagrams at fixed filling exhibit a region of phase separation between SS and SF phases in the small-$U$ large-$V$ regions.

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