Competing Supersolid and Haldane Insulator phases in the extended one-dimensional bosonic Hubbard model

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The Haldane Insulator is a gapped phase characterized by an exotic non-local order parameter. The parameter regimes at which it might exist, and how it competes with alternate types of order, such as supersolid order, are still incompletely understood. Using the Stochastic Green Function (SGF) quantum Monte Carlo (QMC) and the Density Matrix Renormalization Group (DMRG), we study numerically the ground state phase diagram of the one-dimensional bosonic Hubbard model (BHM) with contact and near neighbor repulsive interactions. We show that, depending on the ratio of the near neighbor to contact interactions, this model exhibits charge density waves (CDW), superfluid (SF), supersolid (SS) and the recently identified Haldane insulating (HI) phases. We show that the HI exists only at the tip of the unit filling CDW lobe and that there is a stable SS phase over a very wide range of parameters.

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Since its introduction in 1989 \cite{1}, the bosonic Hubbard model (BHM) has attracted continued interest due to its very rich ground state phase diagram especially in the presence of longer range interactions. Direct experimental relevance was established with the realization of this model Hamiltonian, with tunable parameters \cite{2}, in systems of ultra-cold bosonic atoms loaded in optical lattices \cite{3}. In its simplest form, a single boson species with only contact repulsion, the system exhibits two phases in the ground state \cite{1}, a superfluid (SF) and an incompressible Mott insulator (MI) depending on the particle filling and the interaction strength. Extensive quantum Monte Carlo (QMC) simulations have established that, when longer range interactions are included, the supersolid (SS) phase can form for a wide range of parameters and lattice geometries in one, two and three dimensions \cite{2,4,5,10}. Typically, the SS phase is produced by doping a phase exhibiting long range charge density order (CDW). However, further QMC work has shown that, remarkably, for a wide range of parameters, the extended BHM with near neighbor interactions exhibits a SS phase even at \textit{commensurate} fillings in two and three dimensions \cite{17,18}.

In addition, it was shown that the one-dimensional extended BHM with near and/or near neighbor interactions admits another exotic phase at a filling of one particle per site; the Haldane insulator (HI) \cite{14,20}. The HI is a gapped insulating phase characterized by a highly non-local order parameter like the Haldane phase \cite{21,22} in integer spin chain systems (see below). This gives rise to several questions. 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 \cite{11} 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 \cite{17} and three dimensions \cite{18}? If the SS phase exists for commensurate fillings, where is it situated in the phase diagram relative to the CDW, MI and HI phases? The phase diagram at unit filling for the BHM with contact (U) and near neighbor \textit{(V)} interactions was determined via QMC \cite{23,24} and found to have SF, MI and CDW phases but no SS. Subsequently, the \textit{(µ, t)} phase diagram of the extended BHM, for a fixed \textit{V/U} ratio, was obtained using Density Matrix Renormalization Group (DMRG) \cite{25}, but showed only evidence for MI, SF and CDW phases. More recent work, also based on the DMRG, has found \cite{26} no SS phase in the \textit{(U, V)} plane at unit filling but the question of other fillings was not addressed. Reference \cite{26} also found a HI phase sandwiched between the MI and CDW phases which was not present in \cite{23,24}. As we shall see below, the HI phase was not found in the earlier work because the superfluid density in this phase vanishes very slowly with the system size and the largest sizes that could be accessed at the time were 64 sites.

Theoretical studies of this system using bosonization have led to mixed results. The HI was obtained and characterized with bosonization \cite{20} but consensus is absent on whether the SS phase exists in this model. Even though older studies did not specifically mention it \cite{27} or even argued that it did not exist \cite{28}, more recent studies seem to demonstrate the presence of the SS phase \cite{28}, even without nearest
the chemical potential is targeted by targeting the lowest excitation with the same number of excitations. The neutral gap, \( \Delta_c \), is obtained using DMRG. The charge gap is given by \( \Delta_c \). Several quantities are needed to characterize the phase diagram. The superfluid density is obtained with QMC using

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

where \( W \) is the winding number of the boson world lines, \( d \) is the dimensionality and \( \beta \) the inverse temperature. The CDW order parameter is the structure factor, \( S(k) \), at \( k = \pi \) where

\[
S(k) = \frac{1}{L} \sum_{r=0}^{L-1} e^{ikr} \langle n_0 n_r \rangle,
\]

and the momentum distribution, \( n_k \), is given by

\[
n_k = \sum_{r=0}^{L-1} e^{ikr} \langle a_0^\dagger a_r \rangle.
\]

The charge gap is given by \( \Delta_c(n) = \mu(n) - \mu(n-1) \); the chemical potential is \( \mu(n) = E_0(n+1) - E_0(n) \) where \( E_0(n) \) 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. In both CDW and HI phases, the chemical potentials at both ends are set to (opposite) large enough values, in DMRG, such that the ground state degeneracy and the low energy edge excitations are lifted.

FIG. 1: (color online) Shows several quantities for \( \rho = 1 \) as functions of \( t/U \) with the fixed ratio \( V/U = 0.75 \). (a) The CDW order parameter for \( L = 64 \) and \( \rho_s \), for \( L = 64, 100, 150 \); (b) the parity and string order parameters; (c) the neutral and charge gaps. (a) and (b) were obtained with QMC and (c) with DMRG. The region between the vertical dashed lines is the HI. In the HI, \( \rho_s \rightarrow 0 \) very slowly as \( L \) increases while the string parameter is essentially constant. Note the difference between the neutral and charge gaps. The gaps are given in units of the hopping \( t \).
and therefore, a supersolid phase (SS). The vertical (red) transition is signaled by $\Delta = 0$, and the Fourier transform of $(n_i)$. For the SS phase, $\rho_\perp$ and $\rho_\parallel$ coexist and one expects $\rho_\perp \approx 0$ at the CDW-HI transition. The HI-SF transition, $t/U \approx 0.32$ does not agree with the schematic dashed line in that figure.

As mentioned above, the behavior at $\rho = 1$ may be understood by making the analogy with $S = 1$ spin chains. The question arises as to whether such an analogy between this extended BHM at $\rho = 2, 3, \ldots$ and $S = 2, 3, \ldots$ spin chains is valid and also leads to HI phases. This question is addressed in Fig. 2 for $\rho = 2$ which shows qualitatively different behavior compared to Fig. 1. While for low $t/U$ both cases exhibit CDW phases, the behavior of $\Delta_c$ and $\Delta_n$, calculated with DMRG, is strikingly different as seen in Fig. 2(c): For $\rho = 2$, $\Delta_c = \Delta_n$ and finite size scaling shows that they vanish together at $t/U \approx 0.36$, which indicates that there is no HI in this case. This is consistent with the absence of the Haldane phase in $S = 2$ spin chains [32]. Nonetheless, for this filling, the system does exhibit another salient feature: Indeed, figure 2(a) and (c) show from both QMC and DMRG that when the gaps vanish, $S(\pi)$ remains non-zero while $\rho_\parallel$ also shows a non-zero value. $S(\pi)$ and $\rho_\parallel$ both remain non-zero for $0.33 \leq t/U \leq 0.425$ indicating the presence of a supersolid phase. The CDW-SS transition is estimated to be at $t/U = 0.33$ from QMC and $t/U \approx 0.36$ from DMRG while both DMRG and QMC give $t/U \approx 0.425$ for the SS-SF transition. In Fig. 3 we show $n_k/L$ and $S(k)$ in the SS phase at $t/U = 0.35$ and $L = 64, 100, 128$. We see that while $n_k/L \rightarrow 0$ (see center peak, $k = 0$) as expected (since there is no condensate in one dimension), the peaks in $S(k)$ do not depend on $L$, indicating long range CDW order. This behavior is also confirmed by a finite-size scaling analysis of the DMRG results for sizes $L = 64, 96, 128, 160$. For the three phases (CDW, SS and SF), the CDW order parameter $S(\pi)$ is found to scale as $S_0 + S_1/L + S_2/L^2$, whereas $n_0/L$ is always found to decay as a power law $n_1/L^\alpha$. More precisely, one obtains the following results: for $t/U = 0.25$ (CDW): $S_0 = 3.4$ and $\alpha \approx 0.95$; for $t/U = 0.39$ (SS): $S_0 = 1.6$ and $\alpha \approx 0.22$; for $t/U = 0.49$ (SF): $S_0 \approx 0$ and $\alpha \approx 0.14$. Note that, in both SS and SF phases, the parameter $\alpha$ is less than 0.25, in agreement with a Luttinger liquid description of the system [18, 22, 23]. This scaling law and the insensitivity of $\rho_\parallel$ to $L$, Fig. 2(a), confirm that this is indeed the SS phase. This surprising appearance of the SS phase at commensurate filling has also been observed in two and three dimensions [17, 18]. Furthermore, we find that the Green function, $G(r) = \langle a_r^\dagger a_0 \rangle$, decays as a power in the SS phase with exponent $0.5$ at $t/U = 0.34$.

For the present value of $V/U$, this behavior at $\rho = 2$ is repeated at $\rho = 3$ (and presumably at higher integer fillings): As $t/U$ is increased, the system goes from CDW...
FIG. 3: (color online) The dependence of the momentum distribution, \( n_k/L \) and the structure factor \( S(k) \) on the system size. \( n_k/L \rightarrow 0 \) with increasing \( L \) while \( S(k) \) remains constant indicating long range CDW order.

FIG. 4: (color online) Main panel: The phase diagram of the BHM obtained with QMC and DMRG simulations. All results are for a system with \( V/U = 0.75 \). All symbols are from QMC and are for \( L = 64 \) sites, \( \beta = 128 \) (stars are for \( L = 128 \)). Black lines near the tips of the CDW lobes are DMRG results for \( L = 192 \). The end points of the lobes are obtained by studying the finite size dependence of \( \Delta_n \) using DMRG. The inset is a zoom of the tip of the \( \rho = 1 \) lobe.

Several comments are in order. The \( \rho = 1/2 \) lobe is surrounded almost entirely by SF except for a small region of SS squeezed between it and the \( \rho = 1 \) lobe. The fact that in the extended BHM a SS does not exist when the \( \rho = 1/2 \) CDW phase is doped with holes, but does when it is doped with particles, was already addressed in \cite{11}. The \( \rho = 1 \) lobe sticks out of the SS phase and the part sticking out is, in fact, the HI phase. No other CDW lobe behaves this way. The \( \rho = 3/2 \) lobe terminates right at the boundary with the SF phase: To within the resolution of our simulations, the transition from the \( \rho = 3/2 \) CDW lobe goes directly into the SF phase without passing through the SS phase. This peculiar behavior for \( \rho = 3/2 \) was also observed with additional DMRG results for different values of \( V/U \) ranging from 0.65 to 1: The SS layer between the CDW and SF phases, if present, is too thin to observe for the considered system sizes. An accurate determination of the \((U, V)\) phase diagram for this filling will require a more thorough finite size scaling analysis. All other CDW lobes, \( \rho \geq 2 \), are surrounded entirely by the SS phase. It is interesting to compare this figure with Fig. 3 of \cite{17} and with the mean-field predictions \cite{30}.

In this letter we examined the phase diagram of the extended BHM at a fixed ratio of the interaction terms, \( V/U = 3/4 \). Contrary to expectation, we found that this model at integer fillings does not always behave analogously to integer spin chains. In particular, only for \( \rho = 1 \) and at small \( t/U \) does this happen and the system exhibits CDW, HI and SF phases. In the CDW phase at this filling, \( \Delta_c > \Delta_n \). At all other integer fillings, we found the HI phase to be absent and in its place a supersolid phase which indicates that the system at these fillings may not behave like an integer spin chain. Furthermore, for all CDW phases, except the one at \( \rho = 1 \), we found that \( \Delta_n = \Delta_c \) and that, unlike the \( \rho = 1 \) case, both gaps vanish together as the CDW phase gives way to SS or SF. It is possible that, for a different \( V/U \) ratio, the SS-SF boundary will shift and cut the \( \rho = 3 \) lobe (as it does in Fig. 4 with the \( \rho = 1 \) lobe) resulting in a HI phase. If this happens, it could mean there are two types of \( \rho = 3 \) CDW phases, one in which the neutral...
and charge gaps are always the same (what we find here) and another CDW phase in which $\Delta_c > \Delta_n$ as is the case for the $\rho = 1$ CDW. We have also shown that the single particle Green function decays as a power law in the SS phase. Finally, from a theoretical point of view, it would be interesting to characterize the universality classes of the different quantum phase transitions (CDW-SS-SF) occurring in the system. In addition, in order to have clear experimental signatures of the phases, in particular with cold atom gases which allow time-resolved measurements one would need to study the excitations of the system.

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[37] Note that our definitions of $O_p$ and $O_s$ differ slightly from [19, 20] in that the sum in the exponents is done from $i$ to $j$. This makes $|O_p| = |O_s|$ in the CDW phase for $\rho = 1$. 
