Solitons in Trapped Bose-Einstein condensates in one-dimensional optical lattices

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We use Quantum Monte Carlo simulations to show the presence and study the properties of solitons in the one dimensional soft-core bosonic Hubbard model with near neighbor interaction in traps. We show that when the half-filled Charge Density Wave (CDW) phase is doped, solitons are produced and quasi long range order established. We discuss the implications of these results for the presence and robustness of this solitonic phase in Bose-Einstein Condensates (BEC) on one dimensional optical lattices in traps and study the associated excitation spectrum. The density profile exhibits the coexistence of Mott insulator, CDW, and superfluid regions.

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Localization phenomena in reduced dimensionality take place in a wide range of systems. Shape preserving excitations like lattice solitons, which are intrinsically localized modes, are caused by an interplay of the discreteness of the lattice and non-linearity of the underlying dynamics. These objects have been the focus of intense experimental activity and have been observed in optical waveguide arrays [1], in the quasi one dimensional antiferromagnetic material CuCl [2], and in quasi-one-dimensional Bose-Einstein condensates (BEC) [3]. In this last example, a $\Delta \phi = \pi$ phase flip is imposed on a BEC with repulsive interactions (positive scattering length), exciting a dark soliton. Topological excitations in lattice models of polyacetylene also have a long history [4]. There, localized regions exist in which a transition occurs between two possible configurations of long and short bonds. For reviews, see [5, 6].

Recent effort has focussed on the existence of such localized modes in BEC. Dark solitons were exhibited in numerical solutions to the Gross-Pitaevskii equation [7, 8] while bright solitons were shown to exist in BEC with attractive interactions (negative scattering length) by solving numerically the non-linear Schrödinger equation [9]. In addition, bright solitons are known to exist for repulsive interactions when the effective mass is negative [7] and were shown to exist experimentally for positive scattering length atomic condensates on trapped optical lattices [10]. Since condensate interactions and lattice parameters can be precisely tuned, optical lattices offer the possibility to explore systematically exotic soliton phases. Variational calculations [11, 12] have begun to explore the dynamics and excitations of such systems.

In this paper we use Quantum Monte Carlo (QMC) simulations to determine the effect of near neighbor (nn) repulsive interactions on the ground state phase diagram of BEC on 1d optical lattices, both with and without traps. Our model is the bosonic Hubbard tight binding model,

$$H = -t \sum_i \left( a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i \right) + V_T \sum_i x_i^2 n_i \quad (1)$$

$$+ U \sum_i n_i (n_i - 1) + V_1 \sum_i n_in_{i+1}.$$ 

The hopping parameter, $t$, sets the energy scale, $n_i = a_i^\dagger a_i$ is the number operator, $[a_i, a_j^\dagger] = \delta_{ij}$ are bosonic creation and destruction operators. $V_T$ sets the confining trap curvature, while the contact and near-neighbor interactions are given by $U$ and $V_1$. We use the World Line algorithm and the Stochastic Series Expansion (SSE) method, which work in the canonical and grand canonical ensembles, respectively, and simulate both the soft core ($U$ finite) and hard core cases.

The phase diagram with $V_T = 0$ is known at half filling [13]. For $V_1 < 2t$ the ground state is superfluid while for large $U$ and $V_1 > 2t$ off diagonal long range order is replaced by an incompressible, insulating charge density wave (CDW) phase where sites alternate between high and low occupation. Away from half and integer filling the system is always superfluid. In the hardcore limit, this model can be mapped onto a spinless 1d fermionic model with near-neighbor repulsion and also onto the quantum spin-1/2 XXZ model. The extended 1d fermion Hubbard model (with spin) and the classical spin chain model are both known to have soliton excitations [2, 14]. The main focus of this paper is to demonstrate that solitons continue to exist despite the possibility of multiple occupancy and the presence of a trap.

Static and dynamic quantities like the density and compressibility have already been shown to exhibit unusual features due to the trap, requiring local generalizations of these global quantities [15, 16]. We also show that even more complex spatial structures can exist when the near-neighbor repulsion is nonzero.

To address the question of solitonic excitations, we measure the structure factor at equal imaginary time,

$$S(k) = \frac{1}{L^2} \sum_{x,x'} e^{ik(x-x')} \langle n(x, \tau)n(x', \tau) \rangle,$$ 

where

$$\langle n(x, \tau)n(x', \tau) \rangle = \langle n(x, \tau)n(x', \tau) \rangle - \langle n(x, \tau) \rangle \langle n(x', \tau) \rangle.$$
where $L$ is the number of lattice sites and $0 \leq \tau \leq \beta$. Our simulations are done at $\beta = 10$ which is large enough to study the ground state. To make contact with the excitation spectrum, we use the $f$-sum rule

$$\int_{-\infty}^{+\infty} d\omega \omega S(k, \omega) = N_b E_k,$$

(3)

where $S(k, \omega)$ is the dynamic structure factor ($N_b S(k) = \int d\omega S(k, \omega)$) and

$$E_k = \frac{-t}{L} \langle \cos k - 1 \rangle \langle a_{i+1}^+ a_i + a_i^+ a_{i+1} \rangle |0\rangle,$$

(4)

The dispersion relation is given by the Feynman result,

$$\Omega(k) = \frac{E_k}{S(k)}.$$  

(5)

The dispersion curves shown below are obtained with Eq. 5. However, we have verified that we obtain the same results by measuring the imaginary-time-separated density-density correlation function, performing the Laplace transform using the maximum entropy algorithm to obtain $S(k, \omega)$, and applying Eq. 5 directly.

We first address the uniform, $V_T = 0$, system in the hardcore limit using the SSE algorithm. Figure 1 shows $S(k)$ and $\Omega(k)$ for $L = 128$ sites and two values of $N_b$ off half filling. Note that for small $k$, $\Omega(k)$ for both fillings behaves linearly, indicating phonon excitations and superfluid stability under the Landau criterion. The velocity of sound can be extracted from this small $k$ behavior. Furthermore, the peak at $S(k^*)$, observed at half filling for $k^* = \pi$, and which indicates the CDW order, does not vanish when the system is doped. Instead, its height decreases and $k^*$ shifts to lower values. Corresponding to this quasi-long range order peak in $S(k)$ is a dip in $\Omega(k = k^*)$ giving the soliton excitation energy. This is similar to the roton minimum in two and three dimensions. As the system is doped further, the soliton minimum, and thus quasi-long range order, will disappear. The solitons are also evident in the real space boson density (not shown) in the form of well-localized regions of cross over between the two possible sublattices holding high and low density sites. The presence of soliton excitations in the hardcore system is in agreement with what is known for fermionic and classical spin chains.

The crucial question is whether this behaviour persists for the soft core case which is relevant to atomic condensates on optical lattices. In the soft core case, the contact interaction, $U$, must be large enough to suppress multiple occupancy in order to stabilize the CDW phase at half filling when $V_1$ is large enough. Such large values of $U$ have been achieved experimentally on optical lattices and lead to the Mott phase at full filling. In what follows we fix $U = 5t$. At $V_1 = 4t$, the ground state density profile and correlation function at half filling exhibit a strong CDW pattern. The density-density correlations oscillate with nearly maximal amplitude, indicating quantum fluctuations are small, and show little decay with increasing separation. Doping this system by removing two bosons (Fig. 2) yields pronounced, long-lived, soliton excitations. In real space, as seen in Fig. 2, these appear as local regions of density alternation modulated by an overall ‘beating’ pattern. The beat wavelength (soliton size) is given by $\Delta x = 2\pi/(\pi - k_s)$, where $k_s$ is the position of the soliton energy minimum in $\Omega(k)$. In Fig. 2 we show the dispersion $\Omega(k)$ for several fillings. $S(k)$ behaves like the hardcore case with a peak at $k = k^*$ corresponding to the soliton minimum which moves towards lower $k^*$ as doping is increased. As in the hard-core case, for $N_b < 32$, where the system is superfluid, $\Omega(k) \propto k$ for

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{dispersion_relation}
\caption{The dispersion relation, $\Omega(k)$ and the static structure factor, $S(k)$, vs $k$. Peaks in $S(k)$ at incommensurate wavevectors result in the soliton minima in $\Omega(k)$.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{density_profile}
\caption{The density profile and correlation function (averaged over $10^6$ QMC sweeps) for the doped soft core system.}
\end{figure}
small $k$ showing the stability of the superfluid and the absence of a gap. However, for $N_b = 32$, the system is a gapped CDW insulator. This is seen clearly in Fig. 3 where $\Omega(k)$ goes to a finite value as $k \to 0$. There is also no soliton feature at intermediate $k^\ast$. For $N_b = 32$ the dispersion $\Omega(k)$ has minima only at $k = 0, \pi$.

Placing the system in a trap destroys translational invariance. Nonetheless, we shall now show that robust CDW and solitonic excitations are observed. In Fig. 4 the local density profiles in a trap, $V_T = 0.008$, are given for three fillings. For $N_b = 16$, solitonic oscillations are again evident (see also Fig. 5) as local CDW correlations modulated by a beat envelope. For $N_b = 22$ long range CDW order dominates although some residual solitonic excitations remain near the edges. For $N_b = 55$ one sees a remarkable co-existence of several phases: CDW towards the edges, followed by superfluid (no CDW oscillation and compressible) and then a central incompressible Mott insulator (MI). The density fluctuations in the two CDW regions are decoupled by the intervening MI. Such striking density oscillations have been observed in non-neutral plasmas [17, 18] which, due to their electric charge, have long range repulsive interactions.

Figure 5 shows $\Omega(k)$ for the same fillings as in Fig. 4. For $N_b = 16$ there is a clear solitonic excitation of the
type seen for the uniform system, \( k^* < \pi \). For the higher filling, \( N_b = 55 \), the excitation has shifted towards \( k^* = \pi \) but \( \Omega(k) \) remains relatively high, indicating that this is not true long range order (as is of course clear from the density profile). For \( N_b = 22 \), on the other hand, we see that \( \Omega(k^* = \pi) \) is close to zero indicating the establishment of long range CDW order. Furthermore, there is no evidence of a gap in \( \Omega(k) \) as is seen in the uniform system at half filling (see Fig. 6). The system as a whole is always compressible [15, 16].

Finally, the evolution of the dispersion relation with increasing near-neighbor repulsion is shown for \( N_b = 16 \) in Fig. 6 and \( N_b = 22 \) in Fig. 7. In the former case, a soliton minimum develops, while in the latter case CDW formation takes place instead.

A further interesting feature of Fig. 6 with its solitonic excitations, is the universal crossing of the dispersion curves for different interaction strengths. On the other hand, the crossing in Fig. 7, where CDW order dominates, is not universal. A similar well defined crossing point in the specific heat has been seen both experimentally in \(^3\)He [20] and in fermion Hubbard models [21, 22, 23]. We believe a similar reasoning for the existence of crossing applies here. The integral of the structure factor over all momentum is constrained by the density. Thus if \( S(k) \) increases with \( V_t \) for some momenta (for example at \( k = \pi \) as CDW correlations build up), there must be a corresponding decrease in \( S(k) \) for other momenta. This implies a similar behavior in the dispersion relation \( \Omega(k) \) and hence suggests that dispersion curves for different interaction strengths should cross. As discussed in 22, the universality of the crossing in the specific heat case is a second, and more subtle issue.

In conclusion, we have demonstrated that soliton signatures, which are to be expected in the \( d = 1 \) hard-core boson system owing to its close connection with lattice fermion and spin models, are still very robust when the bosons become soft-core and when they are placed in a confining potential. Rapid progress in the creation of near neighbor repulsion \( V_t \) in optical trap systems suggests that it will soon be possible to look for these solitons experimentally.

We have also found that trapped bosons with near neighbor repulsion can exhibit a remarkably rich density profile in which a Mott insulator at commensurate filling occupied the trap center, followed by a superfluid region and then a CDW region where the density is locally pinned at \( \frac{1}{2} \). This was confirmed by a second, and final superfluid region at the end of the occupied sites. The local compressibility [15, 16] also exhibits some unusual features. We find [19] that the CDW region is the most compressible followed by the SF phase, in sharp contrast to a uniform CDW which has a gap to charge excitations set by the near-neighbor repulsion \( V_t \). Experiments can measure \( S(k) \) and therefore \( \Omega(k) \) [24] which would serve to verify the presence of solitons or other kinds of order. Similarly, as commented earlier, the sound velocity is given by the linear slope at small \( k \).

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