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

F. Hébert,[1] G. G. Batrouni,[1] and R. T. Scalettar[2]
[1]*Institut Non-Linéaire de Nice, Université de Nice-Sophia Antipolis, 1361 route des Lucioles, 06560 Valbonne, France*
[2]*Physics Department, University of California, Davis, California 95616, USA*
(Received 7 December 2004; published 21 June 2005)

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 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.

DOI: 10.1103/PhysRevA.71.063609 PACS number(s): 03.75.Hh, 03.75.Lm, 05.30.Jp

The study of Bose-Einstein condensates (BECs) on optical lattices [1] has opened new doors into studying and understanding the physics of *strongly correlated* quantum systems. Indeed, the strength of the on-site interaction term can be precisely tuned [2], leading to one of the most controllable experimental realizations of a superfluid to Mott insulating (MI) transition [1]. An especially close and quantitative contact has evolved between these experiments and theoretical work on the soft-core bosonic Hubbard model [2]. This has been evident both in the original work in three dimensions and in subsequent studies of very elongated one-dimensional optical lattices [3].

Recently, the first BEC of dipolar atoms (^{52}Cr) was achieved [4]. In this system, the relative strength of the contact and dipole-dipole interactions can be adjusted using one of the 14 observed Feshbach resonances [5]. When this condensate is placed on an optical lattice, the system is governed by the extended bosonic Hubbard model with experimentally *tunable* near-neighbor and even next-near-neighbor interactions [6,7]. Such intersite repulsions can give rise to long-range charge ordering. One of the exciting new possibilities is the experimental realization of exotic phases such as supersolids [8,6] in two dimensions.

In addition to unusual new thermodynamic phases, the ability to tune intersite interactions will make possible the exploration of novel dynamical phenomena in strongly correlated systems. One of the most interesting and important of these is the possibility of the formation of lattice (or gap) solitons. These solitons can be viewed as domain walls between the two degenerate charge density wave (CDW) phases which become the ground states when strong intersite repulsion is present. Such intrinsically localized excitations arising from the interplay of the discreteness of the lattice and nonlinearity of the underlying dynamics have been the focus of intense experimental activity in many different contexts [9–13].

Already, some recent effort has focused on the existence of localized modes in BECs. In the absence of the optical lattice, dark solitons were exhibited in numerical solutions to the Gross-Pitaevskii equation [14] and also observed experimentally [15] while bright solitons were shown to exist in BECs with attractive contact interactions (negative scattering length) by solving numerically the nonlinear Schrödinger equation [16] and observed experimentally [17]. In addition, bright solitons are known to exist for repulsive contact interactions when the effective mass is negative [18] and were shown to exist experimentally for positive scattering length atomic condensates on trapped optical lattices [19]. However, none of these examples are in the strongly correlated regime; they all fall in the domain of the *mean field* where the Gross-Pitaevskii equation gives an accurate description of the system.

In this paper we focus on solitonic excitations in the presence of extended-range interaction in the strongly correlated regime which is not well described by the mean field. We demonstrate soliton formation in a confined strongly correlated system described by the bosonic Hubbard model. In addition, we show that the trapped Bose-Hubbard Hamiltonian with near-neighbor interactions exhibits a rich coexistence of superfluid, charge density wave, and Mott insulator regions as one traverses the system spatially. To this end we use exact quantum Monte Carlo (QMC) simulations to determine the effect of near-neighbor (NN) repulsive interactions on the ground-state phase diagram of a BEC on one-dimensional optical lattices, both with and without traps. The system is described by the bosonic Hubbard tight-binding model,

$$H = -t\sum_i (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) + V_T\sum_i x_i^2 n_i + U\sum_i n_i(n_i-1) + V_1\sum_i n_i n_{i+1}. \qquad (1)$$

The hopping parameter t sets the energy scale, $n_i = a_i^\dagger a_i$ is the number operator, and $[a_i, a_j^\dagger] = \delta_{ij}$ are bosonic creation and destruction operators. V_T sets the confining trap curvature; the contact (U) and near-neighbor (V_1) interactions are determined by the dipolar interactions with the help of Eqs. (2)–(4) in [6]. We use the WORLD LINE QMC algorithm.

The phase diagram with $V_T = 0$ is known at half filling [20]. 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 phase where sites alternate between high and low occupation. Away

1050-2947/2005/71(6)/063609(4)/$23.00

from half and integer filling the system is always superfluid. 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 [21,22].

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

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

where L is the number of lattice sites and $0 \leqslant \tau \leqslant \beta$. 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

$$\int_{-\infty}^{+\infty} d\omega\ \omega S(k,\omega) = N_b E_k, \qquad (3)$$

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

$$E_k = \frac{-t}{L}(\cos k - 1)\langle\Psi_0|\sum_{i=1}^{L}(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i)|\Psi_0\rangle, \qquad (4)$$

The dispersion relation is given by the Feynman result,

$$\Omega(k) = \frac{E_k}{S(k)}. \qquad (5)$$

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. (3) directly.

For solitonic excitations to be possible, 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 [20]. Such large values of U have been achieved experimentally on optical lattices and lead to the Mott phase at full filling [1,3]. 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. 1) yields pronounced soliton excitations. In real space, as seen in Fig. 1, these appear as local regions of density alternation, modulated by an overall "beating" pattern. The beat wavelength (soliton size) is given by $\Delta x = 2\pi/(\pi - k_*)$, where k_* is the position of the soliton energy minimum in $\Omega(k)$. In Fig. 2 we show the dispersion $\Omega(k)$ for several fillings. $S(k)$ (not shown) exhibits a peak at $k=k^*$ corresponding to the soliton minimum [see Eq. (5)] which moves toward lower k^* as doping is increased. For $N_b < 32$, where the system is superfluid, $\Omega(k) \propto k$ for small k, which shows that the low-energy excitations are phonons and that the superfluid satisifes the Landau stability criterion. However, for $N_b=32$, the system is a gapped CDW

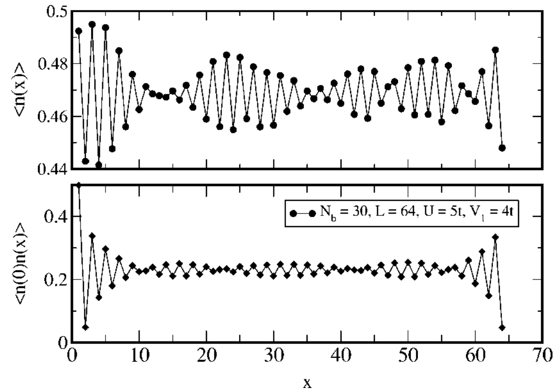

FIG. 1. The density profile and correlation function (averaged over 10^6 QMC sweeps) for the doped soft-core system.

insulator. This is seen clearly in Fig. 2 where $\Omega(k)$ goes to a finite value as $k \rightarrow 0$. There is also no soliton feature at intermediate k^*. 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. 3 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. 4) 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 coexistence of several phases: CDW toward the edges, followed by superfluid (no CDW oscillation and compressible), and then a central incompressible Mott insulator. 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 [23,24] which, due to their electric charge, have long-range repulsive interactions.

Figure 4 shows $\Omega(k)$ for the same fillings as in Fig. 3. 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 toward $k^*=\pi$ but $\Omega(k)$ remains relatively high, indicating that this is not true long-

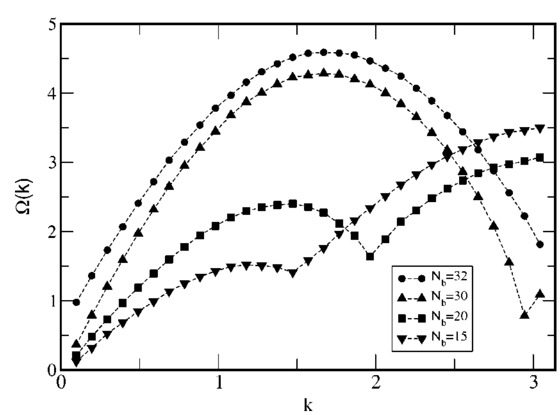

FIG. 2. The dispersion relation $\Omega(k)$ vs k for several fillings for the soft-core model $U=5t$, $V_1=4t$ at $\beta=10$ and $L=64$. Solitons survive despite multiple occupancy.

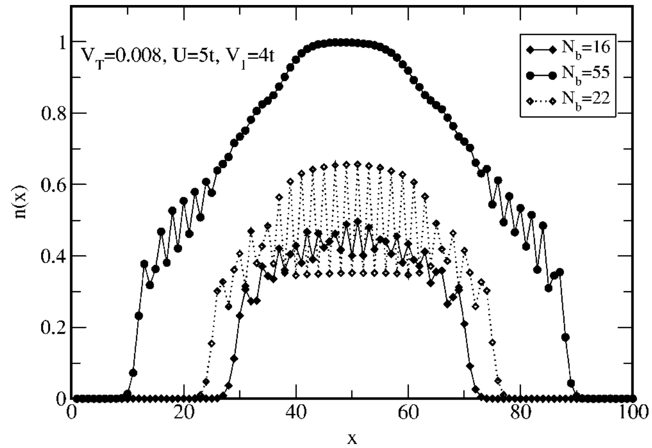

FIG. 3. Density profiles in a trap: For all fillings we see CDW oscillations. For $N_b=22$ the central region has long-range CDW order while for $N_b=55$ the central region is a MI. The $N_b=16$ case exhibits solitonic oscillations.

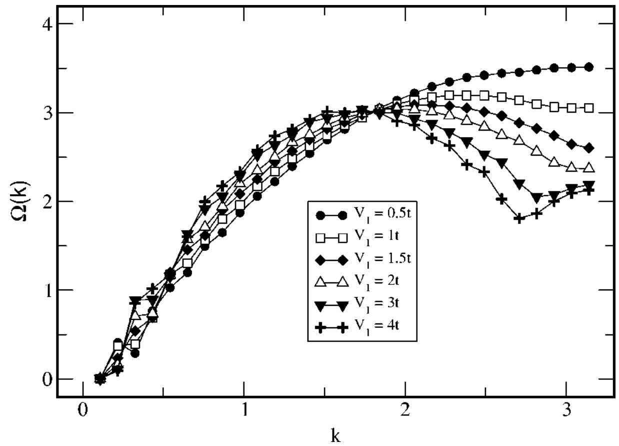

FIG. 5. Evolution of the excitation energy $\Omega(k)$ with increasing V_1 for $U=5t$, $N_b=16$, $V_T=0.008$. The presence of solitonic excitations is clear for $V_1=3t$ and $4t$.

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. For all three densities, $\Omega(k)$ goes to zero as $k\to 0$. This means there is no gap, in contrast to the uniform system at half-filling (see Fig. 2) where $\Omega(k\to 0)$ is nonzero. The absence of a gap implies the system as a whole is always compressible [21,22].

Finally, the evolution of the dispersion relation with increasing near-neighbor repulsion is shown for $N_b=16$ in Fig. 5 and $N_b=22$ in Fig. 6. In the former case, a soliton minimum develops, while in the latter case CDW formation takes place instead.

A further interesting feature of Fig. 5, with its solitonic excitations, is the universal crossing of the dispersion curves for different interaction strengths. On the other hand, the crossing in Fig. 6, 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 [26] and in fermion Hubbard models [27–29]. We believe an analogous reasoning for the existence of crossing applies here. The integral of the structure factor over all momenta is constrained by the density. Thus if $S(k)$ increases with V_1 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 [28] the universality of the crossing in the specific heat case is a second, and more subtle, issue.

In conclusion, we have demonstrated that soliton excitations are present and are very robust in the superfluid phase of the uniform one-dimensional soft-core bosonic Hubbard model with contact and near-neighbor interactions. This Hamiltonian provides an accurate description of confined dipolar atomic BECs in optical lattices [6]. Our results therefore predict that solitons should be experimentally realizable, now that the required near-neighbor interactions can be attained.

We have also found that trapped bosons with near-

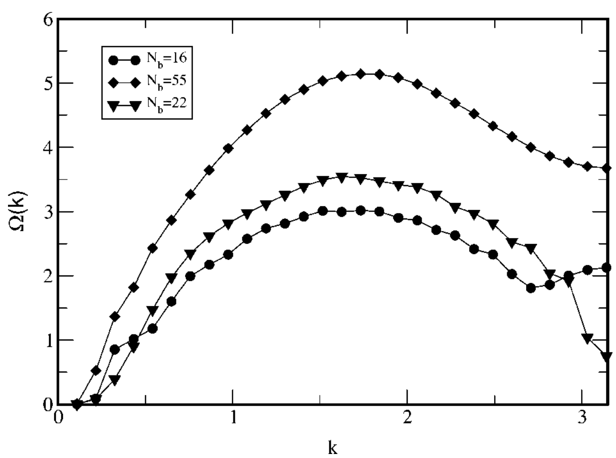

FIG. 4. The excitation energy $\Omega(k)$ vs k for the systems shown in Fig. 3. For $N_b=16$ there is a soliton excitation at $k<\pi$ as in the doped uniform system while for $N_b=22$, $\Omega(k^*=\pi)\to 0$, indicating the establishment of long-range CDW order.

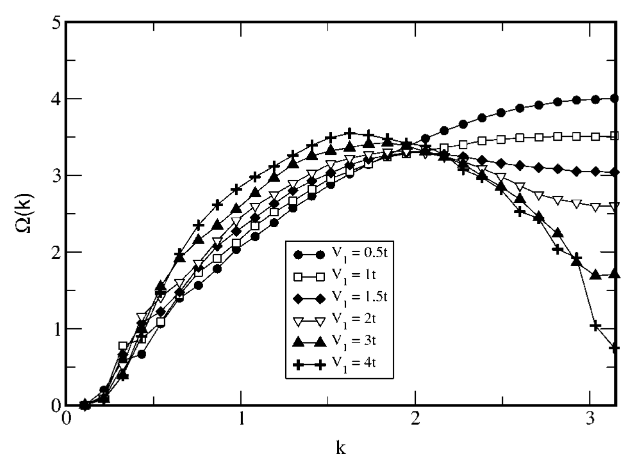

FIG. 6. Evolution of the excitation energy $\Omega(k)$ with increasing V_1 for $U=5t$, $N_b=22$, $V_T=0.008$. The gradual establishment of long-range CDW order is clear.

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 $\frac{1}{2}$, with a second and final superfluid (SF) region at the end of the occupied sites. The local compressibility [21,22] also exhibits some unusual features. We find [25] 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_1. Experiments can measure $S(k)$ and therefore $\Omega(k)$ [30] 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.

The recent realization of such a BEC [4] has now made it very likely that within a very short time confined BECs in optical lattices with tunable near neighbor interactions will be realized. The various phases and excitations discussed here should then be observable with such methods as Bragg spectroscopy [30,31].

We thank R. Kaiser and T. D. Night for very interesting and useful discussions. R.T.S. acknowledges support from NSF Grants No. DMR 0312261 and No. INT 0124863.

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