Quantum bright solitons in a quasi-one-dimensional optical lattice

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We study a quasi-one-dimensional attractive Bose gas confined in an optical lattice with a super-imposed harmonic potential by analyzing the effective one-dimensional Bose-Hubbard Hamiltonian of the system. In order to have a reliable description of the ground-state, that we call quantum bright soliton, we use the Density-Matrix-Renormalization-Group (DMRG) technique. By comparing DMRG results with mean-field (MF) ones we find that beyond-mean-field effects become relevant by increasing the attraction between bosons or by decreasing the frequency of the harmonic confinement. In particular we discover that, contrary to the MF predictions based on the discrete nonlinear Schrödinger equation, average density profiles of quantum bright solitons are not shape invariant. We also use the time-evolving-block-decimation (TEBD) method to investigate dynamical properties of bright solitons when the frequency of the harmonic potential is suddenly increased. This quantum quench induces a breathing mode whose period crucially depends on the final strength of the super-imposed harmonic confinement.

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Ultracold bosonic gases in reduced dimensionality are an ideal platform for probing many-body phenomena where quantum fluctuations play a fundamental role [1, 2]. In particular, the use of optical lattices has allowed the experimental realization [3] of the well-known Bose-Hubbard Hamiltonian [4] with dilute and ultracold alkali-metal atoms. This achievement has been of tremendous impact on several communities [5] since it is one of the first experimental realization of a model presenting a pure quantum phase transition, namely the metal-Mott insulator transition. At the same time new experimental techniques, like in-situ imaging [6], are now available to detect many-body correlations and density profiles. Furthermore, these techniques offer the possibility to observe intriguing many-body effects in regimes which are far from equilibrium. In this contest the relaxation dynamics regimes [7] and light-cone-like effects [8] in a one-dimensional (1D) Bose gas loaded on a optical lattice have been recently observed.

The 1D Bose-Hubbard Hamiltonian, which accurately describes dilute and ultracold atoms in a strictly 1D optical lattice, is usually analyzed in the case of repulsive interaction strength which corresponds to a positive interatomic s-wave scattering length [8]. Indeed, a negative s-wave scattering length implies an attractive interaction strength which may bring to the collapse [10, 11] due to the shrink of the transverse width of a realistic quasi-1D bosonic cloud. Moreover in certain regimes of interaction the quasi-1D mean-field (MF) theory predicts the existence of meta-stable configurations [12] which are usually called discrete bright solitons. We remark that continuous bright solitons have been observed in various experiments [13, 14] involving attractive bosons of $^7$Li and $^{85}$Rb vapors. Instead, discrete (gap) bright solitons in quasi-1D optical lattices have been observed [15] only with repulsive bosons made of $^{87}$Rb atoms.

In this paper we first derive an effective 1D Bose-Hubbard Hamiltonian which takes into account the transverse width of the 3D atomic cloud. In this way we determine a strong inequality under which the effective 1D Bose-Hubbard Hamiltonian reduces to the familiar one and the collapse of discrete bright solitons is fully avoided. We then work in this strictly 1D regime analyzing the 1D Bose-Hubbard Hamiltonian by using the Density-Matrix-Renormalization-Group (DMRG) technique [15]. We evaluate density profiles and quantum fluctuations finding that, for a fixed number of atoms, there are regimes where the MF results (obtained with a discrete nonlinear Schrödinger equation) strongly differ from the DMRG ones. Finally, we impose a quantum quench to the discrete bright solitons by suddenly increasing the frequency of the harmonic potential. By using the time-evolving-block-decimation (TEBD) method [19] we find that this quantum quench induces a breathing oscillation in the bosonic cloud. Also in this dynamical case we find that the MF predictions are not reliable when the on-site attractive energy is large. We consider a dilute and ultracold gas of bosonic atoms confined in the plane $(x, y)$ by the transverse harmonic potential

$$U(x, y) = \frac{m}{2} \omega_x^2 (x^2 + y^2) . \quad (1)$$

In addition, we suppose that the axial potential is the combination of periodic and harmonic potentials, i.e.

$$V(z) = V_0 \cos^2 (2k_0 z) + \frac{1}{2} \lambda z^2 . \quad (2)$$

This potential models the quasi-1D optical lattice produced in experiments with Bose-Einstein condensates by using counter-propagating laser beams [20]. Here $\lambda = \omega_z / \omega_x \ll 1$ models a weak axial harmonic confinement. The characteristic harmonic length is given by
Hamiltonian (in scaled units) and, for simplicity, we choose $a_\perp$ and $\hbar \omega_\perp$ as length and energy unit respectively. We assume that the system is well described by the quantum-field-theory Hamiltonian (in scaled units)

$$H = \int d^3r \psi^+(r) \left[ -\frac{1}{2} \nabla^2 + U(x,y) + V(z) + \pi g \psi^+(r)\psi(r) \right] \psi(r), \quad (3)$$

where $\psi(r)$ is the bosonic field operator and and $g = 2a_s/a_\perp$ with $a_s$ the s-wave scattering length of the interatomic potential \[21\].

We perform a discretization of the 3D Hamiltonian along the $z$ axis due to the presence on the periodic potential. In particular we use the decomposition \[5\]

$$\psi(r) = \sum_i \phi_i(x,y) w_i(z) \quad (4)$$

where $w_i(z)$ is the Wannier function maximally localized at the $i$-th minimum of the axial periodic potential. This tight-binding ansatz is reliable in the case of a deep optical lattice \[22\] \[23\]. To further simplify the problem we set (field-theory extension of the mean-field approach developed in \[11\])

$$\phi_i(x,y)|GS\rangle = \frac{1}{\pi^{1/2}\sigma_i} \exp \left[ - \left( \frac{x^2 + y^2}{2\sigma_i^2} \right) \right] b_i|GS\rangle, \quad (5)$$

where $|GS\rangle$ is the many-body ground state, while $\sigma_i$ and $b_i$ account respectively for the on-site transverse width and for the bosonic field operator. We insert these ansatz into Eq. \[3\] and we easily obtain the effective 1D Bose-Hubbard Hamiltonian

$$H = \sum_i \left\{ \frac{1}{2} \left( \frac{a_{\parallel}^2}{\sigma_i^2} + \sigma_i^2 \right) + V_T \sigma_i^2 \right\} n_i - J b_i^\dagger (b_{i+1} + b_{i-1}) + \frac{1}{2} \frac{U}{\sigma_i^2} n_i (n_i - 1) \right\}, \quad (6)$$

where $n_i = b_i^\dagger b_i$ is the on-site number operator, $\epsilon_i = i^2 V_T$ is the on-site axial energy with $V_T$ the strength (harmonic constant) of the super-imposed harmonic potential, while $J$ and $U$ are the familiar hopping (tunneling) energy and on-site energy which are experimentally tunable via $V_0$ and $a_s$ \[3\]. Even if $J$ and $U$ actually depend on the site index $i$, the choice of considering low $V_T$ allows us to keep them constant. Our Eq. \[4\] takes into account deviations with respect to the strictly 1D case due to the transverse width $\sigma_i$ of the bosonic field. This on-site transverse width $\sigma_i$ can be determined by averaging the Hamiltonian \[3\] over a many-body quantum state $|GS\rangle$ and minimizing the resulting energy function with respect to $\sigma_i$. In this way one gets

$$\sigma_i^2 = 1 + \frac{\langle n_i^2 \rangle - \langle n_i \rangle}{\langle n_i \rangle}, \quad (7)$$

\[8\]

Note that Eqs. \[3\] and \[7\] must be solved self-consistently to obtain the ground-state of the system. Clearly, if $U < 0$ the transverse width $\sigma_i$ is smaller than one (i.e. $\sigma_i < a_\perp$ in dimensional units) and the collapse happens when $\sigma_i$ goes to zero \[11\]. At the critical strength $U_c$ of the collapse all particles are accumulated in few sites and consequently $U_c \simeq -s/N$ (i.e. $U_c/(\hbar \omega_\perp) \simeq -s/N$ in dimensional units) with $s = 1$ if $L$ is odd and $s = 2$ if $L$ is even.

We stress that, from Eq. \[7\], the system is strictly 1D only if the following strong inequality

$$U \frac{\langle n_i^2 \rangle - \langle n_i \rangle}{\langle n_i \rangle} \ll 1 \quad (8)$$

is satisfied for any $i$, such that $\sigma_i = 1$ (i.e. $\sigma_i = a_\perp$ in dimensional units). Under the condition \[3\] the problem of collapse is fully avoided. In the remaining part of the paper we shall work in this strictly 1D regime where the effective Hamiltonian of Eq. \[3\] becomes (neglecting the irrelevant constant transverse energy)

$$H = -J \sum_i (b_i^\dagger b_{i+1} + h.c.) + \frac{U}{2} \sum_i n_i (n_i - 1) + V_T \sum_i i^2 n_i \quad (9)$$

which is the familiar 1D Bose-Hubbard model \[4\].

As already mentioned in a 1D configuration quantum fluctuations, which are actually neglected in mean-field approaches, can play a relevant role. Indeed, as recently shown in an experiment with a Fermi gas at unitarity \[24\] in a cigar-shape configuration, they may bring to strong deviations from mean-field (MF) results. Thus, in our 1D problem it is relevant to compare MF predictions with DMRG ones in order to observe in which regimes MF can give accurate and reliable results. In particular,

\[9\]
we use a MF approach based on Glauber coherent state
\[ |GCS\rangle = |\beta_1\rangle \otimes ... \otimes |\beta_L\rangle \]
whose complex numbers \( \beta_i \) satisfy the 1D discrete nonlinear Schrödinger equation (DNLSE)
\[ \mu \beta_i = V_T t^2 \beta_i - J (|\beta_{i+1} + \beta_{i-1}|^2 + U|\beta_i|^2) \beta_i , \]
where \( \mu \) is the chemical potential of the system fixed by the total number of atoms: \( N = \sum_i |\beta_i|^2 = \sum_i \langle GCS | n_i | GCS \rangle \). By solving Eq. (11) with Crank-Nicolson predictor-corrector algorithm with imaginary time \( 2\theta \), it is possible to show that in the attractive case \( U < 0 \) discrete bright solitons exist \( i \).

On general physical grounds one expects that the MF results obtained from the DNLSE of Eq. (11) are fully reliable only when \( U \to 0 \) and \( N \to \infty \) with \( UN \) taken constant. For this reason, working with a small number \( N \) of bosons it is important to compare the Glauber MF theory with a quasi-exact method. DMRG is able to take into account the full quantum behavior of the system and it has already given strong evidences of solitonic waves in spin chains \( 25 \) and in bosonic models with nearest neighbors interaction. \( 26 \). A crucial point in order to have accurate results by using DMRG is played by the size of the Hilbert space we set in our simulations. Clearly, for system sizes and densities comparable with the experimental ones, we can not investigate the collapse phase where all the bosons "collapse" in one site. Indeed it requires a size of the Hilbert space which is not approachable with our method. Anyway, as shown in Eq. (7), this phase does not happen for sufficiently low density and on-site interaction \( U \). For this reason and in order to fulfill Eq. (7) we consider regimes which are sufficiently far from this scenario, more precisely we use a number \( N = 20 \) of bosons in \( L = 80 \) lattice sites and interactions \( U \geq -0.1 \). Nevertheless if we allow a too small number of bosons per site, namely if we consider a too small Hilbert space, even if we are far from the collapse, our results might be not reliable since the shape of density profile is modified by this cut off and not by physical reasons. To treat this problem we consider a maximum number of bosons in each site \( n_{\text{max}} = 8 \) and we checked that increasing this quantity does not significantly affect our results. Moreover we keep up to 512 DMRG states and 6 fine size sweeps \( 18 \) to have a truncation error lower than \( 10^{-10} \).

In Fig. 1 we compare the density profiles given by DMRG with the ones obtained by using the mean-field DNLSE for different strengths of the harmonic potential and interaction. For weak interactions \( U \) the particles are substantially free and the shape of the cloud is given only by the harmonic strength \( V_T \). Of course when the particles are strongly confined in the center of the system, as in panel a) of Fig. 1, the interaction \( U \) begins to play a role due to the relevant number of bosons lying in the two central sites. More precisely \( U \) tries to drop quantum fluctuations induced by \( J \) and it explains the small but significant discrepancies we find.

When the interaction \( U \) is sufficiently strong (panels g), h), i) of Fig. 1) the MF results becomes insensitive to the super-imposed harmonic potential of strength \( V_T \) since the shape of the cloud remains practically unchanged giving rise to self-localized profiles. Instead DMRG results do not show this self-localization. In fact quantum fluctuations try, in opposition to \( U \), to maximally delocalize the bosonic cloud.

In order to check if our interpretation is valid we plot in Fig. 2 the expectation value of quantum fluctuations
\[ \Delta n_i = \sqrt{\langle n_i^2 \rangle - \langle n_i \rangle^2} . \]
A simple calculation shown that for the Gauuber coherent state \( |GCS\rangle \) one has \( \Delta n_i = \sqrt{n_i} \). We expect that \( \Delta n_i \) of the DMRG ground-state \( |GS\rangle \) can be quite different from the MF prediction. More precisely quantum fluctuations are enhanced by the kinetic term \( J \) which tries to maximally spread the shape of the cloud. On the other hand the value of \( \Delta n_i \) is minimized both by strong on-site interaction because the system gains energy in having as much as particles in the same site and by strong trapping potential which try to confine the bosons in the two central sites of the lattice where the contribute of \( V_T \) is weaker. This behavior is clear in Fig. 2 where, for large \( U \) and small \( V_T \), \( \Delta n_i \) presents strong deviations from MF behavior, whereas mean-field DNLSE and DMRG are in substantial agreement in the opposite regime.

Another relevant aspect of bright solitons is given by its dynamical properties. In particular it is predicted by time-dependent DNLSE \( 12 \) that discrete bright soliton...
can give rise to a breathing mode. To study the time evolution of the system we use the time-evolving-block-decimation (TEBD) algorithm \[14\], which is still a quasi-exact method recently used to study the appearance of a dark soliton \[27\] and its entanglement properties \[28\] \[29\]. We compare TEBD results with time-dependent DNLSE ones, which are immediately obtained from Eq. \[11\] with the position \(\mu \to i \partial / \partial t\). We determine the ground-state of the Bose system for a chosen value \(V_f^{\text{in}}\) of transverse confinement and then we perform the time evolution with a larger value \(V_f\). In this way we mimic a sudden change in the strength \(V_T\) of the super-imposed harmonic confinement (see panel a) of Fig. 3.

In panels b), c), d), e) of Fig. 3 we report the density of atoms in the two central sites (where it takes the highest value since the effect of \(V_T\) is weaker) as a function of time \(t\). The panels show a periodic oscillation where the period \(\tau\) of this breathing mode strongly grows by reducing the harmonic strength \(V_T\). Moreover, \(\tau\) is slightly enhanced by a smaller \(|U|\). Remarkably, as in the static case, beyond-mean-field effects become relevant for a strong \(U\) and they are instead less evident for high values of \(V_T\). Indeed, in Fig. 3 the relative difference between TEBD and MF in the period \(\tau\) is below 1% in panels c) and e), while it is around 8% in panel b) and around 37% in panel d).

In this paper we have shown that for a 3D bosonic system an attractive on-site interaction \(U\) does not automatically imply a collapsed phase and this confirms recent numerical results obtained with dipolar bosons \[31\]. We have obtained indeed a strong inequality, Eq. \[8\], under which the 3D system is reduced to a strictly-1D one and the collapse is fully avoided. Moreover, we have compared MF theory with the DMRG looking for beyond-mean-field effects in the effective 1D system of bosons in a lattice. From our results we conclude that the self-localized discrete bright solitons obtained by the MF nonlinear Schrödinger equation are not found with the DMRG results (quantum bright solitons). In other words, we have found that with a small number \(N\) of bosons the average of the quantum density profile, that is experimentally obtained with repeated measures of the atomic cloud, is not shape invariant. This remarkable effect can be explained by considering a quantum bright soliton as a MF bright soliton with a center of mass \(\mu_0\) that is randomly distributed due to quantum fluctuations, which are suppressed only for large values of \(N\). This is exactly the reasoning adopted some years ago to explain the distributed vorticity of superfluid liquid \(^4\)He \[34\] and, more recently, the Anderson localization of particles in one dimensional system \[35\] and the filling of a dark soliton \[27\]. For the sake of completeness, we have also analyzed the breathing mode of discrete bright solitons after a sudden quench finding that also in the dynamics beyond mean-field effects become relevant for a strong interaction strength \(U\) and for a small harmonic constant \(V_T\). In conclusion, our results give strong evidence on the limitations of MF theory for a small number of bosons. They may help to clarify the impressive and totally new experimental results on nonlinear effects in reduced dimensions, as the ones obtained in \[24\].

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