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We study a quasi-one-dimensional attractive Bose gas confined in an optical lattice with a superimposed harmonic potential by analyzing the one-dimensional Bose-Hubbard Hamiltonian of the system. Starting from the three-dimensional many-body quantum Hamiltonian, we derive strong inequalities involving the transverse degrees of freedom under which the one-dimensional Bose-Hubbard Hamiltonian can be safely used. To have a reliable description of the one-dimensional ground state, which we call a 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 find 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 method to investigate the 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 superimposed harmonic confinement.

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I. INTRODUCTION

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 had a tremendous impact on several communities [5] since it is one of the first experimental realizations of a model presenting a pure quantum phase transition, namely the metal-Mott insulator transition. At the same time, new experimental techniques, such as *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 that are far from equilibrium. In this context, the relaxation dynamics regimes [7] and light-cone-like effects [8] in a one-dimensional (1D) Bose gas loaded on an 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 [9]. Indeed, a negative s-wave scattering length implies an attractive interaction strength, which may bring about a collapse [10,11] due to the shrinking 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 metastable configurations [12], which are usually called discrete bright solitons. We remark that continuous bright solitons have been observed in various experiments [13–16] involving attractive bosons of ^{7}Li and ^{85}Rb vapors. Instead, discrete (gap) bright solitons in quasi-1D optical lattices have been observed [17] only with repulsive bosons made of ^{87}Rb atoms.

In this paper, we first derive an effective 1D Bose-Hubbard Hamiltonian that 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 [18]. 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.

II. THE MODEL

We consider a dilute and ultracold gas of bosonic atoms confined in the plane (x,y) by the transverse harmonic potential

$$U(x,y) = \frac{m}{2}\omega_\perp^2(x^2+y^2). \tag{1}$$

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

$$V(z) = V_0\cos^2(2k_0 z) + \tfrac{1}{2}\omega_z^2 z^2. \tag{2}$$

This potential models the quasi-1D optical lattice produced in experiments with Bose-Einstein condensates by using counterpropagating laser beams [20]. We choose

$\lambda = \omega_z/\omega_\perp \ll 1$, which implies a weak axial harmonic confinement. The characteristic harmonic length of transverse confinement is given by $a_\perp = \sqrt{\hbar/(m\omega_\perp)}$, and, for simplicity, we choose $a_\perp$ and $\hbar\omega_\perp$ as length unit and energy unit, respectively. In the rest of the paper, we use scaled variables.

We assume that the system is well described by the quantum-field-theory Hamiltonian (in scaled units)

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

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

A. Discretization

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]

$$\psi(\mathbf{r}) = \sum_i \phi_i(x,y) w_i(z), \tag{4}$$

where $w_i(z)$ is the Wannier function maximally localized at the ith minimum of the axial periodic potential. In this paper, we consider the case of an even number L of sites $z_i = (2i - L - 1)\pi/(4k_0)$ with $i = 1,2,\ldots,L$.

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])

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

where $|\mathrm{GS}\rangle$ is the many-body ground state, while σ_i and b_i account, respectively, for the adimensional on-site transverse width (in units of $a_\perp$) and the bosonic field operator. We insert this ansatz into Eq. (3) and we easily obtain the effective 1D Bose-Hubbard Hamiltonian

$$H = \sum_i \left\{\left[\frac{1}{2}\left(\frac{1}{\sigma_i^2} + \sigma_i^2\right) + \epsilon_i\right] n_i - J\, b_i^+(b_{i+1} + b_{i-1}) + \frac{1}{2}\frac{U}{\sigma_i^2} n_i(n_i - 1)\right\}, \tag{6}$$

where $n_i = b_i^+ b_i$ is the on-site number operator,

$$\epsilon_i = \int w_i^*(z)\left[-\frac{1}{2}\frac{\partial^2}{\partial z^2} + V(z)\right] w_i(z) dz \tag{7}$$

is the on-site axial energy, which can be written as $\epsilon_i = V_S + V_T\,(2i - L - 1)^2$ with V_S the on-site energy due to the periodic potential and V_T the strength (harmonic constant) of the superimposed harmonic potential, while J and U are the familiar adimensional hopping (tunneling) energy and adimensional on-site energy, which are experimentally tunable via V_0 and a_s [9]. J and U are given by

$$J = -\int w_{i+1}^*(z)\left[-\frac{1}{2}\frac{\partial^2}{\partial z^2} + V(z)\right] w_i(z)\, dz, \tag{8}$$

$$U = g\int |w_i(z)|^4 dz. \tag{9}$$

Remember that now $V(z)$ is in units of $\hbar\omega_\perp$ and z is in units of $a_\perp$. 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.

B. Dimensional reduction

Our Eq. (6) takes into account deviations with respect to the strictly 1D case due to the transverse width σ_i of the bosonic field. We call the Hamiltonian (6) quasi-1D because it depends explicitly on a transverse width σ_i, which is not equal to the characteristic length $a_\perp$ of the transverse harmonic confinement.

This on-site transverse width σ_i can be determined by averaging the Hamiltonian (6) over a many-body quantum state $|\mathrm{GS}\rangle$ and minimizing the resulting energy function,

$$\langle \mathrm{GS}|H|\mathrm{GS}\rangle = \sum_i \left\{\left[\frac{1}{2}\left(\frac{1}{\sigma_i^2} + \sigma_i^2\right) + \epsilon_i\right]\langle n_i\rangle + \frac{1}{2}\frac{U}{\sigma_i^2}\left(\langle n_i^2\rangle - \langle n_i\rangle\right) - J\left(\langle b_i^+ b_{i+1}\rangle + \langle b_i^+ b_{i-1}\rangle\right)\right\} \tag{10}$$

with respect to σ_i. Notice that the hopping term is independent of σ_i. In this way, by using the Hellmann-Feynman theorem, one immediately gets

$$\sigma_i^4 = 1 + U\frac{\langle n_i^2\rangle - \langle n_i\rangle}{\langle n_i\rangle}. \tag{11}$$

Equations (6) and (11) must be solved self-consistently to obtain the ground state of the system. Clearly, if $U < 0$, the transverse width σ_i is smaller than 1 (i.e., $\sigma_i < a_\perp$ in dimensional units) and the collapse happens when σ_i goes to zero [11]. At the critical strength U_c of the collapse, all particles are accumulated in the two central sites ($i = L/2$ and $i = L/2 + 1$) around the minimum of the harmonic potential, and consequently $U_c \simeq -2/N$ [i.e., $U_c/(\hbar\omega_\perp) \simeq -2/N$ in dimensional units].

We stress that, from Eq. (11), the system is strictly 1D only if the strong inequality

$$U\frac{\langle n_i^2\rangle - \langle n_i\rangle}{\langle n_i\rangle} \ll 1 \tag{12}$$

is satisfied for any i, such that $\sigma_i = 1$ (i.e., $\sigma_i = a_\perp$ in dimensional units). Under the condition (12), the problem of collapse is fully avoided.

III. NUMERICAL RESULTS

In the remaining part of the paper, we shall work in this strictly 1D regime where the effective Hamiltonian of Eq. (6)

becomes (neglecting the irrelevant constant transverse energy)

$$H = -J \sum_i b_i^\dagger (b_{i+1} + b_{i-1}) + \frac{U}{2} \sum_i n_i(n_i - 1) + \sum_i \epsilon_i n_i, \tag{13}$$

which is the familiar 1D Bose-Hubbard model [4]. We call the Hamiltonian (13) strictly 1D because the transverse width σ_i is equal to the characteristic length $a_\perp$ of transverse harmonic confinement.

A. Glauber coherent state and DNLSE

As already mentioned, in a 1D configuration, quantum fluctuations, which are actually neglected in mean-field approaches, can play a relevant role. 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, we use a MF approach based on a Glauber coherent state,

$$|\mathrm{GCS}\rangle = |\beta_1\rangle \otimes \cdots \otimes |\beta_L\rangle, \tag{14}$$

where $|\beta_i\rangle$ is, by definition, such that $b_i|\beta_i\rangle = \beta_i|\beta_j\rangle$ [24]. By minimizing the energy $\langle \mathrm{GCS}|H|\mathrm{GCS}\rangle$ with respect to β_i, one finds that the complex numbers β_i satisfy the 1D discrete nonlinear Schrödinger equation (DNLSE)

$$\mu\, \beta_i = \epsilon_i \beta_i - J(\beta_{i+1} + \beta_{i-1}) + U|\beta_i|^2 \beta_i, \tag{15}$$

where μ is the chemical potential of the system fixed by the total number of atoms: $N = \sum_i |\beta_i|^2 = \sum_i \langle \mathrm{GCS}|n_i|\mathrm{GCS}\rangle$. By solving Eq. (15) with the Crank-Nicolson predictor-corrector algorithm with imaginary time [25], it is possible to show that in the attractive case ($U < 0$), discrete bright solitons exist [11].

On general physical grounds, one expects that the MF results obtained from the DNLSE of Eq. (15) are fully reliable only when $U \to 0$ and $N \to \infty$, with UN taken constant. Indeed, the Glauber coherent state $|\mathrm{GCS}\rangle$ is the exact ground state of the Bose-Hubbard Hamiltonian only if $U = 0$ and $N \to \infty$. Notice that the exact ground state of the Bose-Hubbard Hamiltonian with $U = 0$ and a finite number N of bosons is the atomic coherent state $|\mathrm{ACS}\rangle$, which reduces to the Glauber coherent state $|\mathrm{GCS}\rangle$ only for $N \to \infty$ (see, for instance, [26]). In practice, one expects that MF results are meaningful in the superfluid regime where there is a quasicondensate, i.e., algebraic decay of phase correlations [1,5,21]. Nevertheless, in general it is quite hard to determine this superfluid regime. For this reason, working with a small number N of bosons, it is important to compare the Glauber MF theory with a quasiexact method.

B. DMRG approach

DMRG is able to take into account the full quantum behavior of the system, and it has already given strong evidence of solitonic waves in spin chains [27] and in bosonic models with nearest-neighbor interaction [28]. A crucial point in order to have accurate results by using DMRG involves the size of the Hilbert space we set in our simulations. Clearly, for system sizes and densities comparable with the experimental ones, we cannot investigate the collapse phase where all the bosons "collapse" in one site. Indeed, it requires a size of the Hilbert space that is not approachable with our method. In any case, as shown in Eq. (11), this phase does not happen for sufficiently low density and on-site interaction U. For this reason, and in order to fulfill Eq. (11), we consider regimes that are sufficiently far from this scenario. More precisely, we use a number $N = 20$ of bosons in $L = 80$ lattice sites and interactions $U \geqslant -0.1$. Nevertheless, if we allow a too small number of bosons per site, i.e., if we consider a too small Hilbert space, even if we are far from the collapse, our results might not be reliable since the shape of the density profile is modified by this cutoff and not by physical reasons. To treat this problem, we consider a maximum number of bosons in each site, $n_{\max} = 8$, and we checked that increasing this quantity does not significantly affect our results. Moreover, we keep up to 512 DMRG states and six fine size sweeps [18] to have a truncation error lower than 10^{-10}.

C. Comparing DMRG with DNLSE

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 [Figs. 1(g)–1(i)], the MF results become insensitive to the superimposed 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-

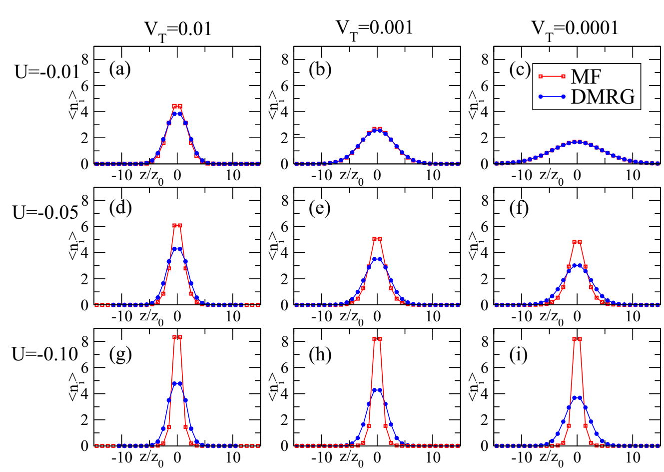

FIG. 1. (Color online) MF (squares) and DMRG (circles) density profiles $\langle n_i \rangle$ of the bright soliton with $J = 0.5$, $L = 80$, and $N = 20$. On the horizontal axis there is the scaled axial coordinate z/z_0, with $z_0 = \pi/(4k_0)$. The results of each panel are obtained with different values of harmonic strength V_T (columns) and interaction strength U (rows).

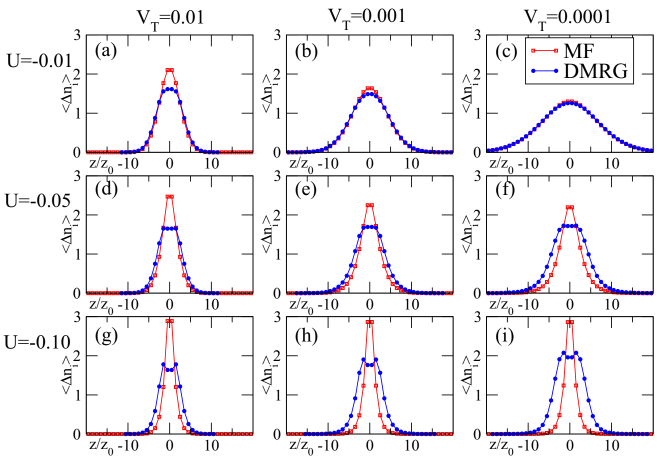

FIG. 2. (Color online) MF (squares) and DMRG (circles) quantum fluctuations $\Delta n_i = \sqrt{\langle n_i^2\rangle - \langle n_i\rangle^2}$ of the bright soliton with $J = 0.5$, $L = 80$, and $N = 20$. On the horizontal axis there is the scaled axial coordinate z/z_0, with $z_0 = \pi/(4k_0)$. The results of each panel are obtained with different values of harmonic strength V_T (columns) and interaction strength U (rows).

localization. In fact, quantum fluctuations try, in opposition to U, to maximally delocalize the bosonic cloud.

To check if our interpretation is valid, we plot in Fig. 2 the expectation value of quantum fluctuations,

$$\Delta n_i = \sqrt{\langle n_i^2\rangle - \langle n_i\rangle^2}. \tag{16}$$

For the Glauber coherent state $|\text{GCS}\rangle$, one has $\Delta n_i = \sqrt{n_i}$. We expect that Δn_i of the DMRG ground state $|\text{GS}\rangle$ 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 Δn_i is minimized both by the strong on-site interaction (because the system gains energy having many particles in the same site) and by the strong trapping potential (which confines the bosons in the two central sites of the lattice where V_T is weaker). This behavior is clear in Fig. 2, where, for large U and small V_T, Δn_i presents strong deviations from MF behavior, whereas mean-field DNLSE and DMRG are in substantial agreement in the opposite regime.

D. Dynamical properties

Another relevant aspect of bright solitons is given by its dynamical properties. In particular, it is predicted by time-dependent DNLSE [12] that a 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 [19], which is still a quasiexact method recently used to study the appearance of a dark soliton [29] and its entanglement properties [30,31]. We compare TEBD results with time-dependent DNLSE ones, which are immediately obtained from Eq. (15) with the position $\mu \to i d/dt$. We determine the ground state of the Bose system for a chosen value V_T^{in} of transverse confinement, and then we perform the time evolution with a larger value V_T^{fin}. In this way, we mimic a sudden change in the strength V_T of the superimposed harmonic confinement [see panel (a) of Fig. 3].

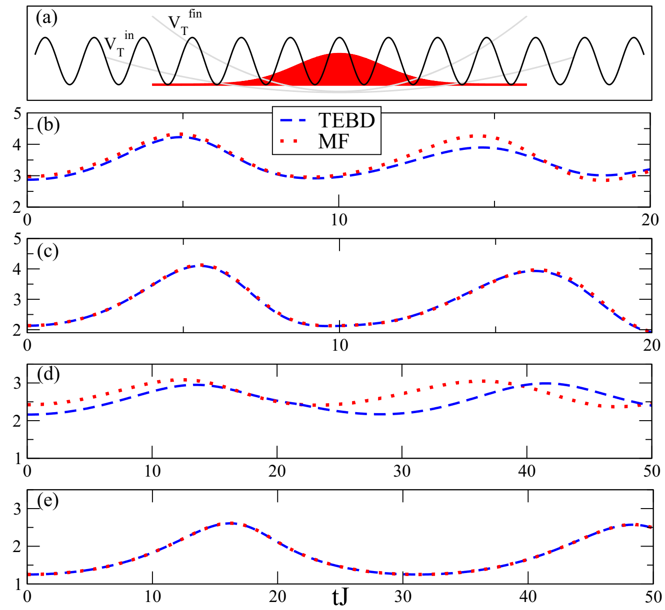

FIG. 3. (Color online) (a) Illustration of the quench procedure. In the other panels: MF (dotted lines) and TEBD (dashed lines) central density $\langle n_{L/2}\rangle$ vs time t with $J = 0.5$, $L = 40$, and $N = 10$. Panels (b) and (c): quench from $V_T^{\text{in}} = 0.01$ to $V_T^{\text{fin}} = 0.05$ for, respectively, $U = -0.1, -0.01$. Panels (d) and (e): quench from $V_T^{\text{in}} = 0.001$ to $V_T^{\text{fin}} = 0.005$ for, respectively, $U = -0.1, -0.01$.

In Figs. 3(a)–3(d), 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 τ of this breathing mode strongly grows by reducing the harmonic strength V_T. Moreover, τ 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 τ is below 1% in panels (c) and (e), while it is around 8% in panel (b) and around 37% in panel (d).

IV. CONCLUSIONS

In this paper, we have obtained a strong inequality, Eq. (12), 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, which is experimentally obtained with repeated measures of the atomic cloud, is not shape-invariant [32]. This remarkable effect can be explained by considering a quantum bright soliton as a MF bright soliton with a center of mass [33,34] that is randomly distributed due to quantum fluctuations, which are suppressed only for large values of N [35]. This is the same kind of reasoning adopted some years ago to explain the distributed vorticity of superfluid liquid ^{4}He [36], and, more recently, the Anderson localization of particles in a one-dimensional system [37] and the filling of a dark soliton [29]. 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 [38]. Our paper presents strong evidence of the limits of MF theory in the study of bright solitons, suggesting that DMRG calculations must be used to simulate and analyze them.

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