Dipole oscillations of confined lattice bosons in one dimension

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We study the dynamics of a non-integrable system comprising interacting cold bosons trapped in an optical lattice in one-dimension by means of exact time-dependent numerical DMRG techniques. Particles are confined by a parabolic potential, and dipole oscillations are induced by displacing the trap center of a few lattice sites. Depending on the system parameters this motion can vary from undamped to overdamped. We study the dipole oscillations as a function of the lattice displacement, the particle density and the strength of interparticle interactions. These results explain the recent experiment C. D. Fertig et al., Phys. Rev. Lett. 94, 120403 (2005).

Recent experiments with cold atoms have provided realizations of non-equilibrium quantum multi-body systems, allowing to address a number of fundamental questions. For example, the integrability of a many-body system has been demonstrated in Ref. [2], via the inhibition of thermalization in a one-dimensional Bose gas, which opened the way to theoretical studies of the relaxation dynamics of non-equilibrium many-body systems [5]. The dynamics of non-integrable systems has been recently explored experimentally in Refs. [3, 4] using interacting cold bosonic atoms trapped in an array of one-dimensional optical lattices and confined by a parabolic potential. Dipole oscillations were induced by displacing the center of the parabolic potential, and the dipole dynamics was studied by monitoring the position of the center of mass. A sudden transition from a regime of undamped motion to a regime of strongly damped motion was observed on increasing the lattice depth. Since damping of the center of mass oscillations is due to excitations in the optical lattice, the results obtained in [3, 4] have provided precious diagnostic of the dynamical correlations of the many-body system, and thus have stimulated considerable theoretical interest [7, 8, 9].

The experiment in [4] was performed in a parameter regime where the use of the following Bose-Hubbard Hamiltonian is microscopically justified [11]:

$$H = -J \sum_j (b_j^\dagger b_{j+1} + \text{h.c.}) + \Omega \sum_j [j + \delta(t)]^2 n_j + \frac{U}{2} \sum_j n_j(n_j - 1).$$

The first term on the r.h.s. of Eq. (1) describes the tunneling of bosons between neighboring sites with rate $J$ ($j$ labels the sites on the lattice). The second term is the parabolic potential with curvature $\Omega$; $\delta(t)$ is a sudden displacement of the trap center, $\delta(t) = \delta(t) \Theta(t)$ (with $\Theta(t)$ the Heaviside function), and $n_j = b_j^\dagger b_j$ is the density operator with bosonic creation (annihilation) operators $b_j^\dagger$ ($b_j$). The last term is the onsite contact interaction with energy $U$. (we set $\hbar = 1$).

The sudden displacement on the trap center causes dipole oscillations of the bosons which can be analyzed experimentally by monitoring the time evolution of the Center Of Mass (COM) $x_{\text{com}} = \sum_j j n_j / N$, with $N$ the number of particles. The experiment of Ref. [4] was performed on a array of one-dimensional optical lattices where the number of particles in each 1D lattice varied from $N \approx 80$ to zero. Thus, in order to provide a comprehensive and quantitative comparison with the experimental data, here we analyze the dipole dynamics as a function of $\delta$, $U/J$, and the number of bosons $N$. We find that overdamped motion can occur as a function of $\delta$ for arbitrarily small interactions, Fig. [8] while in general sizeable interactions tend to extend the parameter region where localization occurs [12]. For a given $\Omega/J$ damping...
is found to depend exponentially on $U/J$, and to be favored for small $N$. Figure 3(a), where the damping rate is shown as a function of the interaction and the number of bosons and, most important, Fig. 3(b), where we compare our numerics with the experimental data finding a very good agreement in the intermediate range of interactions, allow for a new explanation of the experiment of Ref. [4], based on the role of lattices with different $\delta$. (b) Density distribution for $N = 11$ and 15 particles, respectively, for $\Omega/J = 0.05623$. In each panel, the dashed and solid lines are $U/J = 1$ and 20, respectively. The solid line in panel (b) corresponds to a Mott insulator. (c) Density distribution for $N = 23$, $\Omega/J = 0.4$, and $U/J = 1$ and 20 (dashed and solid lines, respectively). The solid line corresponds to a cake-like structure. (d-f) Snapshots of the density distribution for the cases (a-c), with $U/J = 20$ and $\delta = 4$, at times $tJ = 0, 30, 40$ and 50. The dynamics of a few atoms in the Mott and cake-like configurations is frozen, however, residual oscillations can persist in the latter, see text.

Three regimes are of interest for the dipole dynamics [see Fig. 1]: a) for $4J \gtrsim \Omega(N/2)^2$ the density distribution is Gaussian or Thomas-Fermi-like for $4J \gg U$ and $4J \simeq U$, respectively; and for $U \gg 4J$ onsite densities are smaller than one; b) for $U > \Omega(N/2)^2 > 4J$ a Mott insulator with one particle per site is formed at the trap center; c) for $\Omega(N/2)^2 > U > 4J$ a shell structure is formed with a density $1 < n_i \lesssim 2$ at the trap center, surrounded by a Mott-insulator with one particle per site. All the situations above occur in the experiment, since $N$ varies from one lattice to another. Therefore, in the following we are first interested on the dynamics of model systems as those in Fig 1 which exemplify all three cases a), b) and c) above while still allowing for an extensive analysis in terms of all parameters $N, \Omega/J$ and $U/J$, and then we address the experiment of Ref. [3] in the most interesting regime $U/J \gtrsim 4$.

The results presented below have been obtained by means of a tDMRG algorithm with a second order Trotter expansion of $H$, and time-steps $0.01J$ [4]. We take advantage of the conserved total number of particles $N$ projecting on the corresponding subspace; the truncated Hilbert space dimension is up to $m = 100$, while the allowed number of particles per site is $D = 5$. All results below are found to be independent of this choice.

We first focus on the dipole dynamics as a function of the trap displacement $\delta$, in the regime of weak interactions. In this regime, mean-field theory predicts a sudden transition between undamped and overdamped motion via a dynamical instability at a critical displacement $\delta_c \simeq \sqrt{2J/\Omega}$ [12]. This value for $\delta_c$ can be understood by employing the exact solution of Eq. (1) in the non-interacting limit [13]. For energies $E \lesssim 4J$ the single-particle eigenstates of $H(t = 0)$ are harmonic-oscillator-like modes extended around the center of the parabolic trap. However, for $E > 4J$ particles are Bragg-scattered by the lattice, and perform Bloch-like-oscillations centered far from the trap center [14]. The particle localization corresponds to the population of these latter high-energy modes, which becomes significant for displacements $\delta \gtrsim \delta_c$, [13]. Our numerical results in the limit of weak interactions are shown in Fig. 2(a-c), where dipole oscillations of the center of mass $x_{com}$ are shown as a function of time $t$, for different values of the displacement $\delta$. In the simulations, as initial condition we use the ground-state wavefunction of the undisplaced potential, shifted by $\delta$ lattice sites. On increasing $\delta$, the dynamics changes from undamped to damped, and the particles oscillate around the trap center. On increasing further the displacement $[\delta \gtrsim 5$ in panels (a-b)] the oscillations are overdamped, and the COM slowly drifts towards the trap center or clings to the borders of the trap (case with $N = 23$ of panel c)). This behavior corresponds to the localization transition predicted by mean-field theory. However, Fig. 2 shows that quantum fluctuations, properly accounted for by the tDMRG, smear out the transition into a smooth crossover between the undamped and the overdamped regimes.

Having established a connection with known results in the mean-field regime, we now present exact results for the particle localization in the interesting case of stronger interactions $U/J \gtrsim 1$ and $\delta \lesssim \delta_c$. We first focus on model systems and fix $\delta_c = 6$ and the displacement $\delta = 1 < \delta_c$, such that for small interactions $U/J \lesssim 1$ the dynamical instability discussed above does not occur, e.g. for $U/J = 1$ the dipole oscillations are undamped for all $N$, see Figs. 2(a)-(b). The dipole dynamics is then studied as a function of the ratio $U/J$. In particular, Fig. 3(a) shows the damping rate $\Gamma$ of the dipole oscillations as a function of $U/J$ for $N = 11, 15$ and 28 [exemplifying cases a), b) and c) above]. Here, $\Gamma$ is calculated using the expression for underdamped oscillations $x_{com}(t) = e^{-\Gamma t}[1 - \cos(\Omega t + \phi_0)] + y_0$, with $\Gamma$, $\phi_0$ and $y_0$ fitting parameters. Three key observations are in order. i) The damping rate increases exponentially with $U/J$ for intermediate interaction strengths $2 \lesssim U/J \lesssim 6$, a result which is not captured by mean-field, and is signif-
significantly larger than what predicted using phase-slip techniques, valid for $U \lesssim 1$ \cite{12}. ii) Eventually for large enough interactions ($U/J \sim 6$) the oscillations are overdamped for all $N$. We find that for the cases $N = 15$ and 28, this overdamping corresponds to the formation of a Mott-state and a cake-structure as in Fig. 1(b) and (c), respectively. In particular, for $N = 15$ the particle localization occurs for $U/J \approx 4$, a value remarkably close to the superfluid/Mott-insulator quantum phase transition in an homogeneous lattice at commensurate filling and zero current. That is, the results for $\delta < \delta_c$ naturally interpolate between the finite-current dynamical instability and the zero-current quantum phase transition \cite{12}. iii) Despite the Mott-formation for large $N$, for a given $U/J$ the damping $\Gamma$ is actually larger for smaller $N$, such that for $N = 11$ the dynamics is frozen already for $U/J < 4$. In the following we show that this has crucial consequences for the interpretation of the results of Ref. \cite{2} in the most interesting regime of interactions $U/J \sim 4$.

In the experiment of Ref. \cite{4}, the decay of dipole oscillations was studied as a function of the optical lattice depth $V_0$ for a fixed displacement $\delta = 8$, finding damping already for weak lattices $V_0/E_R > 0.5$, with $E_R$ the recoil energy. The experimental data are shown as black dots in Fig. 3(b) as a function of $V_0$ in the range $2 \lesssim V_0/E_R \lesssim 5$, where the use of Eq. (1) is justified \cite{1,12,13}, corresponding to the interesting regime of interactions $3 \lesssim U/J \lesssim 8$. For $V_0/E_R = 3$ and $V_0/E_R > 3$ the value of the damping rate $\Gamma$ has been extracted using formulas appropriate for underdamped and overdamped motion, respectively \cite{4}. The most interesting experimental finding shown in Fig. 3(b) is the measurement of an abrupt transition from a weakly damped regime to an overdamped regime for a lattice depth $V_0/E_R \gtrsim 3$, where the damping rate $\Gamma$ of the dipole oscillations increases by more than an order of magnitude. The physical mechanism behind this apparent transition has proven elusive.

In Fig. 3(b) the experimental results are compared to our numerical results for $N = 80$ and 45, green diamonds and red squares, respectively. The value $N = 80$ has been chosen since it corresponds to the number of particles in the central 1D lattice of the array in the experiment, which is the most largely populated with $\langle n_j \rangle > 1$ for all $U/J$, as in Fig. 1(c). Conversely, the case $N = 45$ exemplifies case (b), with $\langle n_j \rangle \lesssim 1$ for $U/J \gtrsim 4$. The figure shows a very good agreement between the numerical and the experimental results in the entire region $2 \lesssim V_0/E_R \lesssim 5$ ($3 \lesssim U/J \lesssim 8$). However, the case $N = 80$ slightly underestimates the damping around $V_0/E_R \approx 4$, while the agreement for $N = 45$ is almost perfect. For $V_0/E_R \gtrsim 5$ all numerical results fall inside the experimental errorbars, however, the case $N = 45$ shows a strong damping, while the case $N = 80$ falls in the middle of the experimental errorbars. The explanation of the results above stems from the observation that in the experiment $\delta_c$ varies between $\delta_c \sim 18$ and 15 for $3 \lesssim V_0/E_R \lesssim 5$, and thus $\delta < \delta_c$ for all lattice depths. We can then use the results for the model systems of Fig. 3(a) to explain the experimental findings. That is: i) the transition observed experimentally at $V_0/E_R \approx 3$ is actually a crossover, where the 1D systems with the lowest number of particles tend to localize first, in agreement with the discussion of Fig. 3(a). ii) For $V_0/E_R \gtrsim 5$, the dynamics of particles in the 1D systems with $\langle n_j \rangle \lesssim 1$ ($N = 45$ in the simulations) is completely frozen, and the overall mobility of the cloud is due to residual oscillations in lattices with higher onsite density. This latter observation is in agreement with the results of Ref. \cite{11}, where it is shown that for $V_0/E_R > 5$ the damping rate observed in the experiment is well reproduced by the results for $N = 80$. We notice that numerical results for $N = 80$ consistent with ours have been recently reported in \cite{10}, however the focus here is on a comprehensive explanation of the experiment \cite{4}.

The different behaviors of $\Gamma$ for $N = 45$ and 80 and $U/J > 4$ can be modeled as follow. In the low-density case with $N = 45$ the tendency to localization is explained by noting that interactions broaden the spatial width of the atom cloud, until the onsite density falls below one [see also Fig. 1(a-b)]. In this case, the low-energy physics maps into that of an extended cloud of non-
interacting fermions, with single-band Hamiltonian \[^{13}\]

\[
\hat{H}_1(t) = -J \sum_{<i,j>} c_i^\dagger c_j + \Omega \sum_j [j - \delta(t)]^2 c_i^\dagger c_j,
\]

with \(c_j\) and \(c_j^\dagger\) fermionic operators. For large enough displacements \(\delta\), the fermions largely occupy localized modes of the single-particle spectrum discussed above, and the COM remains frozen. The dynamics of interacting particles at large density, e.g. \(N = 80\) in Fig. 3(b), can be modeled starting from the case of largest interactions \(U/J \gg 1\), where the density profile has a cake-like structure, Fig. 4(c). This situation is well described by an extended fermionization model \[^{9, 13, 19}\], where Eq. (1) is replaced by an effective Hamiltonian with two coupled Fermi bands separated by an energy \(U/J\)

\[
\hat{H}_2(t) = -J \sum_{<i,j>} \left[ c_i^\dagger c_j + 2d_j^\dagger d_j + \sqrt{2} (c_i^\dagger d_j + d_j^\dagger c_i) \right] + \sum_j \left[ \Omega [j + \delta(t)]^2 c_j + \{\Omega [j + \delta(t)]^2 + U\} d_j^\dagger d_j \right],
\]

with the operators \(c_j, c_j^\dagger\) and \(d_j, d_j^\dagger\) referring to the lower and higher energy bands of width \(4J\) and \(8J\), respectively. Oscillations in this limit are due to the dynamics of the (delocalized) \(d_j\)-fermions of Eq. (2) in the higher-energy band, while \(c_j\)-fermions are frozen in a (band) insulator. Observing these residual oscillations thus corresponds to probing the superfluidity of bosons with two-particles per site in a homogeneous lattice, in a local-density-approximation sense. \[^{21}\]

This picture, valid for \(U/J \gg 1\) \[^{9, 19}\], can be extended to gain a qualitative insight in the dependence of the dipole oscillations on interactions for \(4 \lesssim U/J \lesssim 10\). In fact, neglecting the parabolic potential, in this regime the model of Eq. (2) suggests that the spectrum is continuum, since the gap \(U\) between the two Fermi bands is smaller than their total width. It is thus plausible that Bloch-like oscillations of the particles are here suppressed, and transport restored. However, for \(U \gtrsim 12J\) the energy spectrum develops a gap again around \(4J\), and thus transport in the lower-energy band is inhibited. Residual current is then due to delocalized particles in the higher-energy band, as explained above. We notice that this picture is consistent with our numerical findings for \(U/J > 5\) in Fig. 3(b).

In conclusion, we have explained the experiment in \[^{4}\] in the most interesting regime of intermediate interactions. The very good agreement between experimental and tDMRG results demonstrates the latter as a unique tool for quantitative comparisons with cold gases experiments in the strongly correlated regime in one dimension.

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\[\text{FIG. 3: (a) Numerical results for the damping rate } \Gamma \text{ of the dipole oscillations vs } U/J \text{ for a fixed displacement } \delta = 1 < \delta_c \text{, with } \delta_c = 6 \Omega/J = 0.05623 \text{ and } N = 11, 15 \text{ and } 28 \text{ cases (a-c) in the text}; (b) Damping rate } \Gamma \text{ for the experiment of Ref. } \[^{4}\] \text{ vs } U/J \text{ and the lattice depth } V_0/E_R. \text{ The experimental data, and the numerical results for } N = 45, 80 \text{ are the black dots, the red squares and the green diamonds, respectively.} \]

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