Monopole excitations of a harmonically trapped one-dimensional Bose gas from the ideal gas to the Tonks-Girardeau regime

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Using a time-dependent modified nonlinear Schrödinger equation (m-NLSE) — where the conventional chemical potential proportional to the density is replaced by the one inferred from Lieb-Liniger’s exact solution — we study frequencies of the collective monopole excitations of a one-dimensional (1D) Bose gas. We find that our method accurately reproduces the results of a recent experimental study [E. Haller et al., Science 325, 1224 (2009)] in the full spectrum of interaction regimes from the ideal gas, through the mean-field regime, through the mean-field Thomas-Fermi regime, all the way to the Tonks-Girardeau gas. While the former two are accessible by the standard time-dependent NLSE and inaccessible by the time-dependent local density approximation (LDA), the situation reverses in the latter case. However, the m-NLSE treats all these regimes within a single numerical method.

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The study of excitations of a material allows us to understand its underlying nature and forms the basis of various spectroscopic methods. In particular, collective excitations of ultracold atoms provide a way to infer their character, including the nature of their interatomic interactions. The goal of this paper is to simulate the monopole oscillations for a Bose gas in a one-dimensional (1D) harmonic oscillator (HO) potential for all range of interaction strengths to demonstrate the continuous transition from the bosonic ideal gas and mean-field regimes at weak interaction to the fermionic strongly correlated limit at large interaction strength. A number of experiments on the excitations of 1D Bose gas exist,$^{[1–3]}$ and yet a unified theoretical description over all interaction regimes has not been available.

So far the experimental regime between Thomas-Fermi and Tonks-Girardeau that shows the crossover of the oscillation frequency from $\omega = \sqrt{3}\omega_z$ to $\omega = 2\omega_z$ has been described by the local density approximation (LDA) combined with sum rules,$^[4]$, while very recently, it was shown that a Hartree approach allows for an accurate description of Gaussian Bose-Einstein condensate (BEC) to Thomas-Fermi regimes that shows the crossover of frequency from $\omega = 2\omega_z$ to $\omega = \sqrt{3}\omega_z$. In the above work, it is further shown that while the two predictions can be joined almost continuously for the cases involving more than 25 particles, $ab\ initio$ diffusion Monte Carlo calculations provide a complete all-regimes data for smaller numbers of atoms. In our Letter, we suggest a simple unified numerical description for macroscopic numbers of atoms in all experimental regimes, using a single wave equation. We compare our results with the findings of a 2009 experiment of Nägerl group$^[2]$ that dealt with ultracold Cs atoms in a 1D harmonic trap. The authors of the experiment tuned the interaction of the 1D ultracold atomic gas via Feshbach resonance while measuring the change in the ratio of the oscillation frequencies of the collective compression ($\omega_C$) and dipole ($\omega_D$) modes, $R = (\omega_C/\omega_D)^2$. This ratio provides the diagnostics for the crossover between different regimes.

Our numerical method of choice is the modified nonlinear Schrödinger equation (m-NLSE), where the conventional chemical potential proportional to the density is replaced by the one inferred from Lieb-Liniger’s exact solution. Our m-NLSE unifies the standard time-dependent NLSE valid in the ideal gas limit and in the neighboring mean-field regime (both before the validity of the Thomas-Fermi approximation and in the Thomas-Fermi regime) and the time-dependent LDA valid for the mean-field Thomas-Fermi regime, Tonks-Girardeau regime, and in between. It should be noted that unlike, for instance, experiments with BECs, not many experiments have so far been performed in the broad area outside of the weakly interacting mean field regime that would allow us to compare and help refine the numerical approach; the experiment of Ref. [2] is a notable exception. Granted, our method is more than a naive interpolation between the standard NLSE at weak interactions and the LDA at the strong ones, since there exists a parameter region—the mean-field Thomas-Fermi regime—of overlapping ranges of validity of the above methods. Nevertheless, more experimental input would help further justify our approach.

Our paper extends Ref. [6] in that we go beyond the steady state solutions and study the dynamics of the harmonically trapped 1D Bose gas over all range of interactions, and differs from Ref. [4] in that we numerically simulate the oscillations directly without resorting to sum rules which give the upper limit to the excitation frequencies calculated based on the static wave functions. It is also important to mention that unlike in [6] and [4], our work goes beyond the local density approximation, and in doing so is able to capture the system’s behavior at very low values of the interaction strength.

For weakly interacting ultracold atoms such as typical experimentally produced BECs, the mean field description of the Gross-Pitaevskii Equation (GPE) has been found to be very effective in describing their collective
oscillations\[7]. More generally, the time-dependent LDA (or hydrodynamical) equations were found to work when the atoms are not necessarily weakly interacting, i.e. beyond mean field\[8,9], and even in the limit of strong correlations of Tonks-Girardeau (TG) regime where the strong interaction between bosons mimic the Pauli exclusion principle so as to make them behave as if they are free fermions\[4].

The time-dependent LDA equations are:

\[
\frac{\partial}{\partial t} n + \nabla (vn) = 0
\]

\[
m \frac{\partial}{\partial t} v + \nabla \left( \mu + V_{\text{ext}}(r) + \frac{1}{2} m v^2 \right) = 0
\]

where \( n \) is the density of gas, \( v \) is the velocity field, \( \mu = \mu[n(r,t)] \) is the local density-dependent chemical potential, \( \mu_i \) is the chemical potential calculated for a uniform gas at density \( n_i(r,t) \), and \( V_{\text{ext}}(r) \) is the external confining potential. It is noted that for weakly interacting BECs with negligible quantum depletion, \( n \) gives the density of the condensate itself (rather than the total density of atoms – condensate plus non-condensates). Physically, LDA typically corresponds to the case of zero temperature, large \( N \) limit, and “macroscopic” dynamics where LDA produced length scales are much larger than both the interparticle distance and the healing length. These conditions, although they superficially appear strict, are found not too difficult to meet in practice.

The excitation of ultracold atoms in the framework of quantum hydrodynamics is modeled analytically by putting all the time-dependence in the deviation from the steady-state value: \( n(r,t) = n_0(r) + \delta n(r,t) \) and \( \mu(r,t) = \mu_1[n_0(r)] + \delta \mu(r,t) \) where \( \delta \mu(r,t) = \left( \frac{\partial \mu_1}{\partial n} \right) |_{n=n_0} \delta n \). The equation to be solved is then \( \delta n = \nabla \left( n \nabla \delta \mu(r,t) / m \right) \) where the double dot denotes the second order time derivative, and from this the corresponding excitation frequencies can be worked out\[5] (see also \[8\] for more details). In order to find the required chemical potential for 1D Bose gas in HO potential encompassing all regimes of quantum correlations, we use the formalism of Lieb and Liniger\[10\] that considers the Hamiltonian with zero range 1D repulsive potentials:

\[
H = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \frac{\partial^2}{\partial z_i^2} + g_{1D} \sum_{i<j}^{N} \delta(z_i - z_j)
\]

A more recent work\[11\] has shown that the interaction strength \( g_{1D} \) is related to the 1D scattering length \( a_{1D} \) as \( g_{1D} = \frac{2 \pi}{m a_{1D}} \) where the interplay between strong interactions and confinement to low dimensional geometry amplifies the effect of quantum correlations, and that given an experimentally relevant cigar-shaped confining trap with longitudinal frequency \( \omega_z \) and transverse frequency \( \omega_\perp \), \( a_{1D} = (-a_\perp^2 / 2a) \left[ 1 - C(a/a_\perp) \right] \), where \( a_\perp = \sqrt{2h/m \omega_\perp} \) is the size of the transverse ground state wave function and \( C = 1.4603 \) is inversely proportional to the actual scattering length \( a \). This means that the strongly correlated beyond mean field regime is approached when the density \( n \) decreases or when \( a_{1D} < d \) where \( d = 1/n \) is the interatomic distance. The chemical potential for this system is calculated using \( \mu_i = \partial [\mu_1(n_i)] / \partial n_i \) where the energy per particle \( \epsilon(n) = \hbar^2 n^2 \epsilon(n) / 2m \) comes from solving the Lieb-Liniger system of equations that arise from applying the Bethe Ansatz\[14\]; here, \( \gamma(n) \) is the dimensionless Lieb-Liniger interaction parameter proportional to the interaction strength \( g_{1D} \), \( \gamma(n) = 2/n(a_{1D}) \).

In the 1D mean field and TG regimes the ground state of the LDA (or hydrodynamical) equations can be found analytically. In the mean field limit of \( n a_{1D} \gg 1 \), \( \gamma \to 0 \) leading to the well known Thomas-Fermi (TF) energy functional; there, the chemical potential is given by \( \mu(n) \approx g_{1D} n = \hbar^2 n^2 / m \). We therefore refer to the 1D mean field limit as the TF limit. In the TG limit of \( n a_{1D} \ll 1 \) where \( \gamma \to \infty \), the chemical potential is \( \mu(n) \approx \pi^2 h^2 n^2 / 2m \). In between the TF and TG limits the chemical potential has to be worked out numerically from the Lieb-Liniger system of equations\[10\] for each \( \gamma(n) \), as exact analytical expression cannot be obtained. Near the TG limit a more accurate analytical approximation for \( \mu(n) \) can be obtained via large \( \gamma \) expansion methods\[10\]:

\[
\mu(n) \approx \frac{\pi^2 \hbar^2}{2m} \left( n \right)^2 \left[ 2 + 3\gamma(n) \right] \left( 3[2 + \gamma(n)] \right)^3.
\]

For comparison with experiments, it is convenient to define the effective \( \gamma \) instead of \( \gamma(n) \) via the maximum steady state density of the atomic cloud at \( z = 0 \) in the TG limit and the actual \( a_{1D} \):

\[
\gamma_{\text{eff.}} = \frac{2}{n_{\text{TG}}(0) |a_{1D}|^3} = \frac{\pi}{\alpha}
\]

where \( n_{\text{TG}}(0) = \sqrt{2N m \omega_z / \hbar^2 \pi} \) is the analytical TG density in the center of the trap\[6\], and for convenience we defined dimensionless parameter \( \alpha = \sqrt{N m \omega_z / 2 \hbar |a_{1D}|} \) that parametrizes the regimes of interaction strength. This naturally introduces a set of \( \gamma \) independent of the density profile, and we shall use \( \gamma_{\text{eff.}} \) as our parameter in our simulation. In Fig.\[1\] the chemical potential per atom, \( \mu(\gamma_{\text{eff.}}) / N \) in HO energy units \( (\hbar \omega_z) \) calculated from the Lieb-Liniger system of equations\[10\] is presented as a function of \( \log_{10} \gamma_{\text{eff.}} \). The near TG formula of Eq.\[1\] is also shown in the figure as a comparison. It is found that the general shape of \( \mu(\gamma_{\text{eff.}}) / N \) is independent of the number of atoms \( N \), and it is seen that as \( \gamma_{\text{eff.}} \to \infty \), \( \mu / N \to 1 \) as to be expected for the TG limit. The analytical expression of Eq.\[1\] is seen to be a good approximation for \( \gamma > 10 \) and also for \( \gamma < 0.01 \).

For simulation purposes, we turn the time-dependent LDA equations Eqs.\[1\] and\[2\] into modified non-linear Schrödinger Equation (n-NLSE) for the wave function \( \Psi(r,t) = \sqrt{n(r,t)} e^{i \Phi(r,t)} \), where we write the density \( n(r,t) = |\Psi(r,t)|^2 \) and the velocity field
\[ \psi(r, t) = \nabla \Psi(r, t) \] 

Here, the standard NLSE nonlinear term, \( g_{1D} |\Psi(r, t)|^2 \Psi(r, t) \) is replaced by \( \mu(n = |\Psi(r, t)|^2) \Psi(r, t) \). For sufficiently smooth density distributions, the two equations are equivalent. Furthermore, besides being better numerically tractable (e.g., the sharp edges of the atomic clouds are automatically regularized), the m-NLSE offers the following benefit. At very low densities, where the size of the cloud become comparable to the size of the one-body quantum ground state of the trap, the time-dependent LDA fails while the standard NLSE is naturally valid there; but this is exactly what the m-NLSE converts to. Thus, the m-NLSE allows for a formal numerical unification of the two regimes.

Note that while at the ideal gas point and in the subsequent mean-field regime, the m-NLSE correctly describes the density evolution at all length scales, in the strongly correlated regime, the m-NLSE must be regarded merely as a simulator for the time-dependent LDA equations, and any features of a healing length size or smaller must be treated as artifacts of the computational method. This question is discussed in Ref.14: it is shown in particular that the interference fringes produced by the m-NLSE in the TG regime have nothing to do with reality.

We are going to work with a wavefunction \( \psi(r, t) = N^{-1/2} \Psi(r, t) \) normalized to unity, \( \int_{-\infty}^{+\infty} |\psi|^2 dz = 1 \), and, accordingly, with a probability distribution \( n = n/N = |\psi|^2 \). Also, in our case, the external potential is given by a one-dimensional harmonic potential \( V_{\text{ext}}(r) = \frac{1}{2}m\omega_z^2 r^2 \). Accordingly, we are going to work in the harmonic oscillator system of units: \( \hbar = m = \omega = 1 \). The m-NLSE equation becomes

\[ i \frac{\partial \psi(z)}{\partial t} = \left[ -\frac{1}{2} \frac{\partial^2}{\partial z^2} + \frac{1}{2} z^2 + \mu[\tilde{n}(z, t)] \right] \psi(z) \]  

where the chemical potential is given by

\[ \mu[\tilde{n}(z, t)] = \frac{N^2}{2} \tilde{n}^2 \left( 3 + \frac{\partial}{\partial \tilde{n}} \right) e(\gamma(n = N\tilde{n})) \]  

calculated numerically from the Lieb-Liniger system of equations[10] at each spatio-temporal step as \( \tilde{n}(z, t) \) evolves.

The simulation was done by first finding the ground state solution for various values of \( \alpha \) starting from the ground state for a HO \( (N = 0) \) and adiabatically increasing \( N \) up to the desired number of atoms. Once the steady state solutions are found, the monopole excitation can then be simulated in many different ways, including an addition by hand of the exact Bogoliubov excitation modes or sinusoidal driving of the confining potential. In this paper, we directly excite monopole oscillations by suddenly quenching the confining potential, from \( V(z) = \frac{1}{2}m\omega_z^2 z^2 \) to \( V(z) = 1.25 \times \frac{1}{2}m\omega_z^2 z^2 \) for some short time \( (\tau = 0.25\pi/\omega_z) \) then back in the original trap frequency. The simulation was then run until \( \tau = 400\pi/\omega_z \) while measuring the time-dependent width (variance) of the wave function

\[ \langle \Delta z^2 \rangle = \int z^2 |\psi(z, t)|^2 dz - \left[ \int |\psi(z, t)|^2 dz \right]^2 . \]  

It was found that except for a short transient, the width \( \langle \Delta z^2 \rangle \) follows a sinusoidal variation over time, owing to the harmonic confining potential. From this sinusoidally varying time-dependent width, the Fourier frequency components were obtained numerically. We have confirmed our procedure outlined above, particularly with respect to finding the steady state solutions, the quenching method to excite monopole oscillations, and the accuracy of the frequency measurement, by carrying out our simulation using Eq. 4 as the chemical potential and finding excellent agreement with the full \textit{ab initio} many-body calculation prediction for the monopole oscillation frequency near the TG limit[13] given by

\[ \left( \frac{\omega_C}{\omega_D} \right)^2 = 2 - \frac{1}{\gamma_{\text{eff.}}} \frac{192}{45\pi} + O \left( \frac{1}{\gamma_{\text{eff.}}}^2 \right) . \]  

We plot in Fig. 2 the steady state density \( n_{ss}(z) \) with atom number \( N = 25 \) for \( \gamma_{\text{eff.f.}} \approx 0.01, 1 \), and \( \gamma_{\text{eff.f.}} \rightarrow \infty \) and the corresponding chemical potential \( \mu(z) \). The position-dependent chemical potential gives an idea of the effective potential experienced by the wave function due to interatomic interaction. This function was found to almost vanish for \( \gamma_{\text{eff.f.}} < 1 \), leaving an effectively interaction-free system of atoms. We also plot the steady state harmonic oscillator energy \( E_{\text{HO}} = \int \psi^*(z) \left[ -\frac{1}{2} \frac{\partial^2}{\partial z^2} + \frac{1}{2} z^2 \right] \psi(z) dz \), the interaction energy \( E_I = \int \psi^*(z) \mu(z) \psi(z) dz \), and the total energy \( E_K + E_I \) as a function of \( \log_{10}(\gamma_{\text{eff.f.}}) \). Additionally, we plot as a function of \( \log_{10}(\gamma_{\text{eff.f.}}) \) the initial, maximum and minimum width of the wave function \( \langle \Delta z^2 \rangle \) attained during the monopole oscillation. It is not surprising that the initial width of the wave function follows the trend of the total energy of the system as a function of \( \gamma_{\text{eff.f.}} \), since the increasing repulsion between the atoms makes the wave function profile wider. The amplitude of oscillation
is seen to also grow as a function of $\gamma_{\text{eff}}$; however taking into account the change in the initial width itself the oscillation amplitude remains constant at approximately 20% of the initial width regardless of $\gamma_{\text{eff}}$.

Experimentally, the group of N"agerl started with a BEC of between $1 \times 10^4$ to $4 \times 10^4$ Cs atoms and by using 2D optical lattice that forms an array of vertical tubes, trapped them in about 3000 to 6000 1D tubes with 8 to 25 atoms in the center tube. Our numerical simulation parameters are within the range of experimental parameters: we cover the same range of $\gamma_{\text{eff}}$ as in the experiment and we use $N = 25$. In Fig. 3 we plot the experimentally measured frequencies ($\omega_C/\omega_D$) with error bars as a function of $\gamma_{\text{eff}}$, and superpose the results from our simulation as well as the prediction. The near-ideal gas region corresponds to the frequency interval from $(\omega_C/\omega_D)^2 \approx 4$ to 3. The point $(\omega_C/\omega_D)^2 \approx 3$ ($\gamma \approx 1$) is the mean-field Thomas-Fermi point. For higher $\gamma_{\text{eff}}$, the system slowly approaches a TG plateau of $(\omega_C/\omega_D)^2 \approx 2$. The sum rule formula of Ref. [4], which was built using LDA, works well in both mean-field Thomas-Fermi and in the TG regimes, but naturally fails for the near-ideal gas. Our approach however captures it.

In conclusion, we found—using a direct comparison with the experimental data[2]—that using a single trivially modified nonlinear Schr"odinger equation one can consistently simulate the 1D Bose gas in the full spectrum of interaction regimes from the ideal gas, through the mean-field regime, through the mean-field Thomas-Fermi regime, all the way to the Tonks-Girardeau gas. While the former two are accessible by the standard time-dependent NLSE and inaccessible by the time-dependent local density approximation (LDA), the situation reverses in the latter case. At the same time, the m-NLSE treats all these regimes using a single numerical method. In addition, it is also interesting to note here that the hydrodynamic simulation was found to agree very well with the results of many-body calculation that considers essentially microscopic oscillations in the near TG limit[13]. As is usually the case in developing viable theoretical models, more experiments are needed to be done and compared with our NLSE to establish the range of validity of our approach. However, many experimental situations involving large amplitude motion, such as problems in quantum transport should satisfy the LDA and hence render the NLSE of Eqs. (6) and (7) a fully valid theoretical model.

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