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 (MNLSE)—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 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-Giradeau gas. While the former two are accessible by the standard time-dependent NLSE and inaccessible by the time-dependent local density approximation, the situation *reverses* in the latter case. However, the MNLSE is shown to treat 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 Letter 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.

Previous work by various authors in describing 1D Bose gas all have involved either some form of nonlinear Schrödinger equation (NLSE) or the equivalent hydrodynamic formulation which are intimately connected via the Madelung transformation as we discuss below. It is found that these have generally been fragmented in terms of the applicable range of interactions. For weakly interacting 1D Bose gas, the 1D Gross-Pitaevskii equation (GPE) applies, with the coupling constant given by $g_{1\mathrm{D}}=-(2\hbar^2/ma_{1\mathrm{D}})$, where $a_{1\mathrm{D}}=(-a_\perp^2/2a)[1-C(a/a_\perp)]$ is the 1D scattering length (negative for repulsive 3D interactions and weak transverse confinement, i.e., for $0 < a < Ca_\perp$), $a_\perp = \sqrt{2\hbar/m\omega_\perp}$ is the size of the transverse ground state wave function, $\omega_\perp$ is the frequency of the transverse confinement, $C \equiv -\zeta(1/2) = 1.4603, \ldots,$ and $\zeta(z)$ is Riemann's zeta function [4]. The above expression takes into account a possibility of a virtual excitation of higher modes in the confining direction at the moment of a two-body collision. For the case when the mean-field potential becomes comparable to the transverse excitation quanta, Salasnich *et al.* [5] derive a cubic NLSE that includes the effect of "spilling" of the transverse component of the 3D GPE wave function to higher transverse modes. It is found that the resulting equation can describe both the weakly interacting mean field and strongly interacting high density Thomas-Fermi (TF) 1D bosons, but not the strongly interacting low atom density Tonks-Girardeau (TG) regime. For the TG regime where interacting impenetrable bosons in 1D behave as noninteracting fermions, a higher nonlinearity than the usual cubic one of GPE is required, and Kolomeisky *et al.* [6] derive a NLSE that includes quintic nonlinearity. It is notable that Minguzzi *et al.* [7] derived from the quintic NLSE of Kolomeisky *et al.* [6] Landau's hydrodynamic equation that matches the well-known result for noninteracting Fermi gas in the hydrodynamic regime [8].

In general, the hydrodynamic equations were found to work beyond the mean field [9,10], including the TG regime [11]. The hydrodynamic equations are

$$\frac{\partial}{\partial t} n + \boldsymbol{\nabla}(\mathbf{v}n) = 0, \tag{1}$$

$$m\frac{\partial}{\partial t}\mathbf{v} + \boldsymbol{\nabla}\left(\mu + V_{\mathrm{ext}}(\mathbf{r}) + \frac{1}{2}m\mathbf{v}^2\right) = 0, \tag{2}$$

where n is the density of gas, $\mathbf{v}$ is the velocity field, $\mu = \mu_l[n(\mathbf{r},t)]$ is the local density-dependent chemical potential, μ_l is the chemical potential calculated for a *uniform* gas at density $n(\mathbf{r},t)$, and $V_{\mathrm{ext}}(\mathbf{r})$ is the external confining potential. The hydrodynamic equations involve the local density approximation (LDA) that corresponds to the case of zero temperature, large N limit, and "macroscopic" dynamics where length scales are much larger than both the interparticle distance and the healing length. These conditions, although they superficially appear strict, are found to be not too difficult to meet in practice. We point out here that the connection between the hydrodynamic equations and NLSE is well established [12,13]. In going from NLSE to the equivalent hydrodynamic formulation, an additional quantum pressure term, $\boldsymbol{\nabla}[-(\hbar^2/2m\sqrt{n})\boldsymbol{\nabla}^2\sqrt{n}]$, is necessarily introduced in Eq. (2). For sufficiently smooth density distributions, such a quantum pressure term is inconsequential on length scales that are much larger than the characteristic microscopic length scales of the problem (such as the healing length, or mean interparticle separation), and the NLSE and the hydrodynamic equations are practically and computationally equivalent in such cases.

Some of us [14] used the hydrodynamic equations to study the stationary state of 1D Bose gas in HO potential from the mean field to the TG regimes via the calculation of required chemical potential encompassing all regimes of quantum correlations. In order to find the chemical potential, the Lieb-Liniger Hamiltonian with zero range 1D repulsive potentials, $\hat{H} = -(\hbar^2/2m)\sum_{i=1}^{N}(\partial^2/\partial {z_i}^2) + g_{1\mathrm{D}}\sum_{i<j}^{N}\delta(z_i - z_j)$, was used to calculate the chemical potential for this system using $\mu_l = \partial[n\epsilon(n)]/\partial n$ where the energy per particle $\epsilon(n) = \hbar^2 n^2 e(\gamma(n))/2m$ comes from solving the Lieb-Liniger system of equations that arises from applying the Bethe *ansatz* [15]. Here, $\gamma(n)$ is the dimensionless Lieb-Liniger interaction parameter proportional to the interaction strength, $g_{1\mathrm{D}}$: $\gamma(n) = 2/n|a_{1\mathrm{D}}|$.

Öberg and Santos [16] and Pedri *et al.* [17] extended Ref. [14] to study the free expansion of 1D Bose gas when the harmonic trap is released, by converting the hydrodynamic equations to a NLSE via the inverse Madelung transform [12,13]. The work of Ref. [16] was limited to a narrow interaction regime between TF and TG, as characterized by the interaction parameter $\eta = n_{\mathrm{TF}}^0|a_{1\mathrm{D}}| \approx 1$ where $n_{\mathrm{TF}}^0 = [(9/64)N^2|a_{1\mathrm{D}}|/a_z^4]^{1/3}$ is TF density with $a_z = \sqrt{\hbar/m\omega_z}$. In addition, owing to the specific form of the *ansatz* for their wave function, it is not *a priori* obvious whether the work may be extended beyond free expansion that they studied. Indeed, more sophisticated experiment beyond free expansion, in particular, that of measuring the monopole oscillation frequency from the mean field to the TG regime, has been performed [2], where the interaction of 8–25 ultracold Cs atoms trapped in an effectively 1D harmonic trap was tuned via the Feshbach resonance while measuring the change in the ratio of the oscillation frequencies of the collective compression (ω_C) and dipole (ω_D) modes, $R = (\omega_C/\omega_D)^2$, the change of which provides the diagnostics for the crossover between different regimes.

So far the experimental regime between TF and TG that shows the crossover of the oscillation frequency has been described by the hydrodynamic equations combined with sum rules [11] which calculate the *upper limit* to the excitation based on the static wave functions. The sum rules method, however, cannot simulate directly the *dynamics* of the 1D Bose gas. Very recently, it was shown that a Hartree approach allows for an accurate description of Gaussian Bose-Einstein condensate to TF regimes and is shown to join smoothly to the crossover from TF to TG described using LDA for the cases involving more than 25 particles [18]. It is further shown that *ab initio* diffusion Monte Carlo calculations provide a complete all-regimes data for the cases involving less than 25 atoms.

These limitations are expected to be overcome in time with, for instance, improved numerical methods and more powerful computers. In this Letter, we show how we overcame these limitations using the modified NLSE (MNLSE) by the inverse Madelung transform, starting with the hydrodynamic equations and adding in the quantum pressure term as we discussed above for mathematical consistency. To obtain MNLSE, the standard NLSE nonlinear term $g_{1\mathrm{D}}|\Psi(\mathbf{r},t)|^2\Psi(\mathbf{r},t)$ is replaced by $\mu(n = |\Psi(\mathbf{r},t)|^2)\Psi(\mathbf{r},t)$. Working with a wave function $\psi(\mathbf{r},t) = N^{-1/2}\Psi(\mathbf{r},t)$ normalized to unity, $\int_{-\infty}^{+\infty}|\psi|^2 dz = 1$, and, accordingly, with a probability distribution $\tilde{n} = n/N = |\psi|^2$ and the external potential given by a one-dimensional harmonic potential $V_{\mathrm{ext}}(\mathbf{r}) = \frac{1}{2}m\omega_z^2 z^2$, the modified MNLSE in the harmonic oscillator system of units, $\hbar = m = \omega = 1$, is

$$i\frac{\partial\psi(z)}{\partial t} = \left[-\frac{1}{2}\frac{\partial^2}{\partial z^2} + \frac{1}{2}z^2 + \mu[\tilde{n}(z,t)]\right]\psi(z), \qquad (3)$$

where the chemical potential is given by $\mu[\tilde{n}(z,t)] = (N^2/2)\tilde{n}^2[3 + \tilde{n}(\partial/\partial\tilde{n})]e[\gamma(n = N\tilde{n})]$, calculated numerically from the Lieb-Liniger system of equations [15] at each spatiotemporal step as $\tilde{n}(z,t)$ evolves. We note that these equations have indeed been obtained earlier [16]. In terms of the validity of the MNLSE, from the mathematical assumptions made, the equation should be valid for all situations where both the LDA and the Lieb-Liniger theory hold. It is noted additionally that throughout the whole range of the interaction strength, the quantum pressure term is either exact (as in the ideal gas and in the GPE regimes, the regime of no interactions, and the regime of weak but non-negligible interactions, the latter thanks to the presence of Bose-Einstein condensate) or negligible (as in the Tonks-Girardeau regime, the regime of strong interactions).

We note that in the mean-field limit of $na_{1\mathrm{D}} \gg 1$, $\gamma \to 0$ leading to the well-known TF energy functional; there, the chemical potential is given by $\mu(n) \approx g_{1\mathrm{D}}n = \gamma\hbar^2 n^2/m$. In the TG limit of $na_{1\mathrm{D}} \ll 1$ where $\gamma \to \infty$, the chemical potential is $\mu(n) \approx \pi^2\hbar^2 n^2/2m$. In between the TF and TG limits the chemical potential has to be worked out numerically. For comparison with experiments, it is convenient to define the effective γ 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},

$$\gamma_{\rm eff} = \frac{2}{n_{\rm TG}(0)|a_{1D}|} = \frac{\pi}{\alpha},$$

where $n_{\rm TG}(0) = \sqrt{2Nm\omega_z/\hbar}/\pi$ is the analytical TG density in the center of the trap [14], and for convenience we defined the dimensionless parameter $\alpha = \sqrt{Nm\omega_z/2\hbar}|a_{1D}|$ that parametrizes the regimes of interaction strength. This naturally introduces a set of γ independent of the density profile, and we shall use $\gamma_{\rm eff}$ as our parameter in our simulation.

The simulation was done by first finding the ground state solution for various values of α starting from the ground state for a HO, i.e., zero effective chemical potential $\mu[\tilde{n}(z,t)]$ in Eq. (3) with $N = 0$ and adiabatically increasing N up to the desired number of atoms. The idea follows from the well-known quantum mechanical theorem on adiabatic following [19], which is the limiting case of the Landau-Zenner transition with zero transition probability such that a system remains in the state that evolves from the initial state in the limit of infinitely slow evolution of the time-dependent Hamiltonian. This turned out to be a crucial numerical step since the strong nonlinearity makes the direct numerical solution to the ground state, i.e., not via some kind of variational *ansatz*, difficult. In this case, the imaginary time evolution or the damping method [20] to obtain the ground state was also found to run into convergence problems, possibly due to the highly nonlinear energy landscape. The fact that the adiabatic following method works well indicates that MNLSE may be applied to simulations involving general trapping potential other than harmonic, as long as the corresponding noninteracting ground state is known.

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 Letter, 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, $\langle\Delta z^2\rangle = \int z^2|\psi(z,t)|^2 dz - [\int z|\psi(z,t)|^2 dz]^2$. 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 plot in Fig. 1 the steady state density $n_{ss}(z)$ with atom number $N = 25$ for $\gamma_{\rm eff} \approx 0.01$, 1, and $\gamma_{\rm eff} \to \infty$ 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 $\gamma_{\rm eff} < 1$, leaving an effectively interaction-free system of atoms. We also plot the steady state harmonic oscillator energy $E_{\rm HO} = \int \psi^*(z)[-\frac{1}{2}(\partial^2/\partial z^2) + \frac{1}{2}z^2]\psi(z)dz$, interaction energy $E_I = \int \psi^*(z)\mu(z)\psi(z)dz$, and the total energy $E_K + E_I$ as a function of $\log_{10}\gamma_{\rm eff}$. Additionally, we plot as a function of $\log_{10}\gamma_{\rm eff}$ 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 $\gamma_{\rm eff}$ 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 $\gamma_{\rm eff}$; 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 $\gamma_{\rm eff}$.

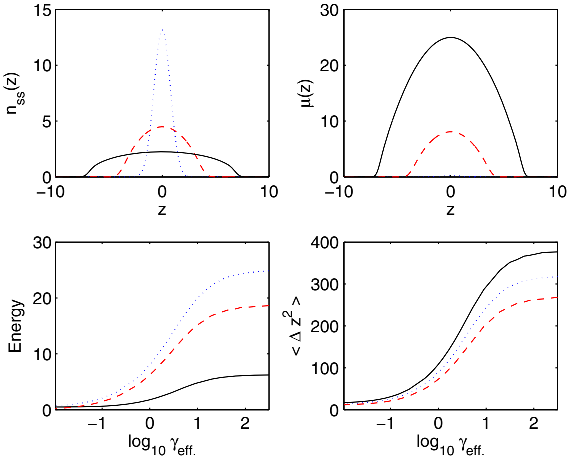

FIG. 1 (color online). Top left panel: plot of the steady state density $n_{ss}(z) = |\psi(z)|^2$ vs z with atom number $N = 25$ for $\gamma_{\rm eff} \approx 0.01$ (dotted line), 1 (dashed line), and $\gamma_{\rm eff} \to \infty$ (solid line). Top right panel: the corresponding chemical potential $\mu(z)$. It is noted that $\mu(z)$ for $\gamma_{\rm eff} \approx 0.01$ (dotted line) is vanishingly small. Bottom left panel: plot of the harmonic oscillator energy $E_{\rm HO}$ (solid line), interaction energy E_I (dashed line), and the total energy $E_K + E_I$ (dotted line) as defined in the text as a function of $\log_{10}\gamma_{\rm eff}$. Bottom right panel: the initial width of the wave function $\langle\Delta z^2\rangle$ (dotted line), minimum $\langle\Delta z^2\rangle$ (dashed line), and maximum $\langle\Delta z^2\rangle$ (solid line) attained during the monopole oscillation as a function of $\log_{10}\gamma_{\rm eff}$. The harmonic oscillator units are used throughout.

Our numerical simulation parameters are within the range of experimental parameters: we cover the same range of $\gamma_{\rm eff}$ as in the experiment and we use $N = 25$. In Fig. 2 we plot the experimentally measured frequencies $(\omega_C/\omega_D)^2$ with error bars as a function of $\gamma_{\rm eff}$ 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

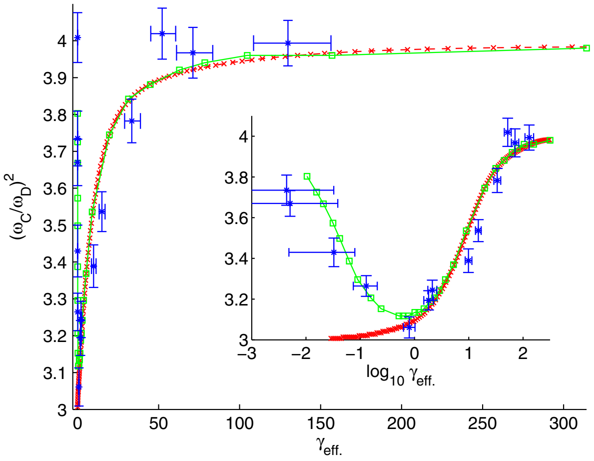

FIG. 2 (color online). Plot of the monopole oscillation frequency squared $(\omega_C/\omega_D)^2$ as a function of $\gamma_{\mathrm{eff}} = 2\pi/\sqrt{2Nm\omega_z/\hbar}|a_{1D}|$. Inset: same figure as a function of $\log_{10}\gamma_{\mathrm{eff}}$ to magnify the region near $\gamma_{\mathrm{eff}} \approx 0$—the region that lies *outside* of the range of validity of hydrodynamic equations. Stars with error bars: the experimental data from the Nägerl group [2]. Green squares: numerical simulation, red crosses: sum rules result [11]. It must be mentioned that in the region of $\gamma_{\mathrm{eff}} \ll 1$, the result [11] is not expected to match the experiment since it has been built on the hydrodynamic equations *a priori*. The difference may be understood from the fact that the effect of the quantum pressure term added in deriving the MNLSE becomes more significant in the regime of weak interactions.

the mean-field TF point. For higher γ_{eff}, the system slowly approaches a TG plateau of $(\omega_C/\omega_D)^2 \approx 2$. The sum rule formula of Ref. [11], which was built using hydrodynamic equations, works well in both mean-field TF and in the TG regimes, but naturally fails for the near-ideal gas. Our approach, however, captures it. The difference may be understood from the fact that the effect of the quantum pressure term added in deriving the MNLSE becomes more significant in the regime of weak interactions.

We note that the sum rules do not necessarily require LDA; the only calculation available for meaningful comparison, Ref. [11], just happens to be built on LDA as they were more interested in the $\gamma \to \infty$ region. 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 TF regime—of *overlapping ranges of validity* of the above methods. Note that while at the ideal gas point and in the subsequent mean-field regime, the MNLSE correctly describes the density evolution at all length scales; in the strongly correlated regime, the MNLSE must be regarded merely as a simulator for the time-dependent LDA equations which is convenient since one does not have to simultaneously track the velocity field and the density—it suffices to track a single wave function, 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. [21]: it is shown, in particular, that the interference fringes produced by the MNLSE in the TG regime [6] have nothing to do with reality.

In conclusion, we found that using a single MNLSE one can consistently simulate the 1D Bose gas in the full spectrum of interaction regimes. Besides being numerically tractable (e.g., the sharp edges of the atomic clouds are automatically regularized), the MNLSE offers the following benefit: at very low densities, where the size of the cloud becomes 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 MNLSE converts to and so MNLSE is able to capture the system's behavior at very low values of the interaction strength. This allows for a formal numerical unification of the standard time-dependent NLSE that is valid in the ideal gas limit and in the neighboring mean-field regime (both before the validity of the TF approximation and in the TF regime) and the time-dependent LDA that is valid for the mean-field TF regime, TG regime, and in between.

The MNLSE bridges the gap between existing previous work from Refs. [4–6,11,14], and [16], each of which has restricted range of applicability. Also, unlike Refs. [11] and [14], the dynamics can be simulated directly. The numerically intensive diffusion Monte Carlo method reported very recently can simulate over all interaction regimes but is restricted to small number of atoms [18]. Furthermore, the adiabatic following method for the ground state preparation implies potential for application of MNLSE to a broad range of future research. On the other hand, we reiterate that there are certain obvious limitations of the MNLSE-hydrodynamic approach such as that discussed by Girardeau and Wright in Ref. [21], which have to do with phenomena at healing length scales.

In general, one may safely apply the MNLSE wherever the LDA holds; many experimental situations involving large amplitude motion, such as problems in quantum transport, should satisfy the LDA and, hence, render the MNLSE a fully valid theoretical model. Although the range of validity of MNLSE is clear from considering the underlying mathematical assumptions, it is also possible that, just as GPE with its theoretically narrow range of applicability (zero temperature, mean field) found wide applications, the MNLSE may have a broader applicability than expected [22]. In this sense, more experiments are needed to be done and compared with our MNLSE to establish the range of validity. On a more fundamental level, since MNLSE is a numerical tool for simulating the hydrodynamic equations, future research should involve careful examination of the validity of the hydrodynamic equations themselves, along the lines of Refs. [23,24].

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