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Exact numerical simulations of a one-dimensional trapped Bose gas

Bernd Schmidt and Michael Fleischhauer
Fachbereich Physik, Technische Universität, Kaiserslautern, D-67663 Kaiserslautern, Germany

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We analyze the ground-state and low-temperature properties of a one-dimensional Bose gas in a harmonic trapping potential using the numerical density-matrix renormalization group. Calculations cover the whole range from the Bogoliubov limit of weak interactions to the Tonks-Girardeau limit. Local quantities such as density and local three-body correlations are calculated and shown to agree very well with analytic predictions within a local-density approximation. The transition between temperature-dominated to quantum-dominated correlation is determined. It is shown that despite the presence of the harmonic trapping potential, first-order correlations display, over a large range, the algebraic decay of a harmonic fluid with a Luttinger parameter determined by the density at the trap center.

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Stimulated by the recent experimental progress in generating ultracold trapped quantum gases in one dimension [1–6] there is a growing interest in correlation dynamical properties of these systems. The physics of one-dimensional (1D) quantum gases is distinct from that in higher dimensions as it is dominated by quantum fluctuations. In a homogeneous system of bosons there is no long-range order even at $T=0$; correlations decay as a power law due to zero-point phase fluctuations. At any finite T there is an asymptotic exponential decay. The most peculiar property of interacting bosons in one dimension is the transition to the fermionlike Tonks-Girardeau gas [7,8] for small densities or large interactions. The transition is characterized by a single effective interaction parameter, the Tonks parameter γ, where small values correspond to the weak interaction or Bogoliubov limit and large values to the Tonks-Girardeau limit. The homogeneous gas is exactly solvable by Bethe ansatz for $T=0$ [9] and finite T [10]. Correlation properties can, however, not easily be extracted from the Lieb-Liniger solution [11] and require, in general, numerical techniques such as Monte Carlo simulations [12]. Approximate analytic expressions can be obtained only for small distances [13] or within the harmonic-fluid approach [14,15].

In the presence of a trap potential $V(x)$ integrability is lost. Nevertheless, in order to calculate local properties Bethe-ansatz solutions for the homogeneous gas are employed together with a local-density approximation (LDA) [16]. Recently we have used stochastic simulation to calculate the density and first-order correlations of a 1D Bose gas in a harmonic trap [17]. The simulations were, however, limited to temperatures larger than the trap energy $k_B T \approx \hbar\omega$ and thus did not allow us to go deeper into the quantum regime. In the present paper we develop an alternative numerical approach based on the density-matrix renormalization group (DMRG) [18,19], which leads to results with much higher precision for temperatures from zero to $\hbar\omega$.

Consider a 1D Bose gas with delta interaction in a (harmonic) trapping potential $V(x)$,

$$\hat{H} = \int dx\, \hat{\Psi}^\dagger(x)\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x) + \frac{g}{2}\hat{\Psi}^\dagger(x)\hat{\Psi}(x)\right]\hat{\Psi}(x), \tag{1}$$

where we have used oscillator units, i.e., $\hbar=m=1$. g is the 1D interaction strength proportional to the s-wave scattering length in one spatial dimension a_{1D} [21].

In the absence of an external trapping potential the Hamiltonian (1) is integrable in the thermodynamic limit, i.e., it has an infinite number of constants of motion. The ground-state solution for $T=0$, which can be obtained by Bethe ansatz [9], shows that the 1D Bose gas is fully characterized by the so-called Tonks parameter $\gamma=g/\rho$. Here ρ is the density of the gas. The Bethe ansatz leads to the so-called Lieb equation for the density of quasimomenta $\sigma(k)$,

$$\sigma(k) - \frac{1}{2\pi}\int_{-1}^{1} dq \frac{2\lambda\sigma(q)}{\lambda^2 + (k-q)^2} = \frac{1}{2\pi},$$

where λ is an implicit function of γ: $\lambda=\gamma\int_{-1}^{1} dk\sigma(k)$. All local properties of the gas can be expressed in terms of the (even) moments of $\sigma(k)$,

$$\epsilon_m(\gamma) = \left(\frac{\gamma}{\lambda}\right)^{m+1}\int_{-1}^{1} dk\, k^m \sigma(k), \quad m=2,4,\ldots.$$

For example, the equation of state reads $\mu=\mu(\rho,g)=g^2 f(\gamma)$,

$$f(\gamma) = \frac{3\epsilon_2(\gamma) - \gamma\epsilon_2'(\gamma)}{2\gamma^2}. \tag{2}$$

Integrability is no longer given when a (harmonic) trapping potential $V(x)$ is taken into account. An often-used approximation to describe the local properties in this case is the LDA. The LDA assumes that the homogeneous solution holds with the chemical potential μ replaced by an effective, local chemical potential $\mu_{\rm eff}(x)=\mu-V(x)$. As long as the characteristic length of changes is small compared to the healing length, the LDA is believed to work well. Within this approximation one finds, e.g., for the density of the gas,

$$\rho(x) = \frac{g}{f^{-1}\left(\frac{\mu_{\text{eff}}(x)}{g^2}\right)}, \qquad (3)$$

where f^{-1} is the inverse function of Eq. (2).

In order to develop, in principle, an exact numerical algorithm we employ powerful real-space renormalization methods such as the DMRG [18,19]. To this end it is necessary to map the continuous to a lattice model. As shown in Refs. [17,22], this can be done in a consistent way by introducing an equidistant grid $x_j = j\Delta x$, $j \in \mathbb{Z}$, which amounts to replacing the field operator $\hat{\Psi}(x_j)$ by $\hat{a}_j/\sqrt{\Delta x}$, where $\hat{a}_j$ is a bosonic annihilation operator. Δx should be chosen small compared to the average distance of particles in order to capture the continuous structure of $\hat{\Psi}$, i.e., $\Delta x \ll \rho^{-1}$. On the other hand, Δx has to be larger than the 1D scattering length $a_{1\text{D}}$. Integrals are replaced by sums and the second derivate in the kinetic energy can be approximated by the difference quotient $\frac{\partial^2}{\partial x^2}\hat{\Psi}(x_j) \approx [\hat{\Psi}(x_{j+1}) + \hat{\Psi}(x_{j-1}) - 2\Psi(x_j)]/\Delta x^2$. This leads to the discretized Hamiltonian, which is equivalent to a Bose-Hubbard Hamiltonian

$$\hat{H} = \sum_j \left[-J(\hat{a}_j^\dagger \hat{a}_{j-1} + \hat{a}_j^\dagger \hat{a}_{j+1}) + D_j \hat{a}_j^\dagger \hat{a}_j + \frac{U}{2}\hat{a}_j^{\dagger 2}\hat{a}_j^2 \right], \qquad (4)$$

with effective tunneling $J = \frac{1}{2\Delta x^2}$, effective energy $D_j = \frac{1}{\Delta x^2} + V(x_j) - \mu$, and effective nonlinear energy given by $U = \frac{g}{\Delta x}$. Expressing the scaled hopping in terms of the Tonks parameter at the trap center, $J/U = 2/\gamma\rho(0)\Delta x \sim \gamma^{-1}$, the 1D gas corresponds to a compressible phase of the Bose-Hubbard model with negative effective chemical potential approaching the line $\mu_{\text{BH}}/U = -2J/U$. In the limit $\Delta x \ll \rho^{-1}$ Hamiltonians (1) and (4) become equivalent.

The numerical DMRG calculations of the density profile, shown in Fig. 1, for Tonks parameters γ ranging from 0.4 to about 70 show excellent agreement with the Lieb-Liniger result with LDA (3) apart from a very small region at the trap edges and the barely visible Friedel-type oscillations, which result from the finite number of particles [20]. One recognizes the typical change of the density profile from an inverted parabola in the Bogoliubov regime $\gamma \ll 1$ to the square root of a parabola in the Tonks-Girardeau limit $\gamma \gg 1$ [21].

An important consequence of the fermionlike behavior of bosons in the Tonks limit $\gamma \gg 1$ is a dramatic reduction of the loss rate due to inelastic three-body collisions [3]. The rate is proportional to the local three-particle correlation $g_3(x) = \langle \hat{\Psi}^{\dagger 3}(x)\hat{\Psi}^3(x)\rangle/\rho(x)^3$, and determines the stability of the Bose gas. Making use of the Hellman-Feynman theorem and the constants of motion of the homogeneous gas Cheianov [25] has found

$$g_3 = \frac{3}{2\gamma}\epsilon_4' - \frac{5\epsilon_4}{\gamma^2} + \left(1 + \frac{\gamma}{2}\right)\epsilon_2' - 2\frac{\epsilon_2}{\gamma} - \frac{3\epsilon_2\epsilon_2'}{\gamma} + \frac{9\epsilon_2^2}{\gamma^2}. \qquad (5)$$

Figure 2 shows a comparison between the numerical data for $g_3(0)$ at the trap center with Eq. (5) and the asymptotic expression in the Tonks-Girardeau limit with the γ taken at the trap center $\gamma(0) = g/\rho(0)$. One recognizes again excellent agreement except for a small deviation for very large γ, where the numerics is, however, susceptible to errors due to the smallness of g_3.

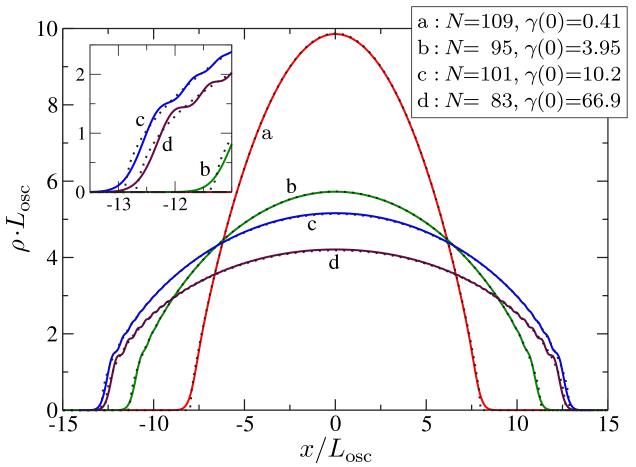

FIG. 1. (Color online) Density of the 1D bosonic gas in a trap at $T=0$. The solid lines are the DMRG results and the dotted lines are the Lieb-Liniger prediction in local-density approximation. Increasing values of γ correspond to decreasing densities at the trap center. The inset shows details at the edge of the density distribution. $L_{\text{osc}} = \sqrt{\hbar/m\omega}$ is the oscillator length corresponding to the trap potential.

In contrast to local quantities, such as the moments of the number density, information about spatial correlations of the homogeneous 1D Bose gas such as $g_1(x_1, x_2) = \langle \hat{\Psi}^\dagger(x_1)\hat{\Psi}(x_2)\rangle/\sqrt{\rho(x_1)\rho(x_2)}$ cannot straightforwardly be obtained from the Lieb-Liniger and Yang-Yang theories. Making use of the asymptotic properties of the Lieb-Liniger wave function for large momenta, Olshanii and Dunjko derived the lowest-order terms of the Taylor expansion of g_1 [13],

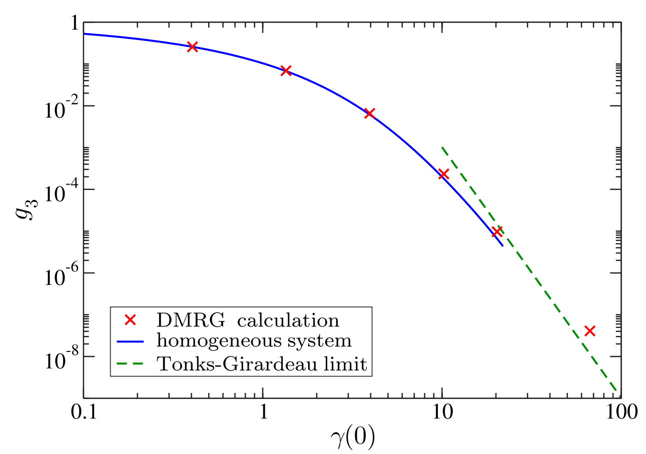

FIG. 2. (Color online) Local third-order correlations as a function of the Tonks parameter at the trap center as obtained from the DMRG calculation (red crosses) compared to the prediction from the Lieb-Liniger theory with the local-density approximation (solid line) and the Tonks-Girardeau limit (dashed line). Parameters of the DMRG calculations are the same as in Fig. 5.

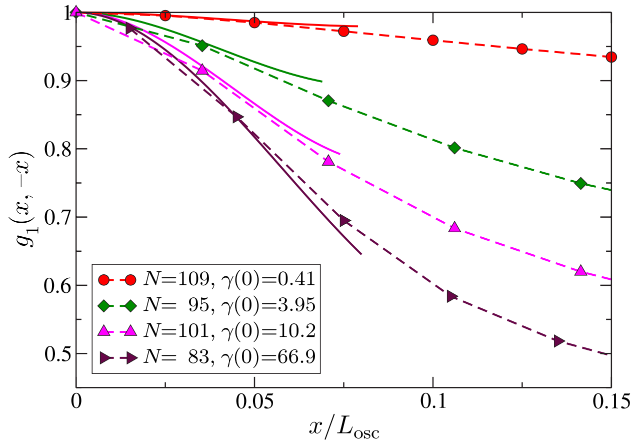

FIG. 3. (Color online) First-order correlations (dashed lines) compared to analytic short-distance expansion (solid lines) for a homogeneous gas with γ taken at the trap center. Values of γ increase from the top to the bottom curve.

$$g_1(x_1,x_2) = 1 - \frac{1}{2}[\epsilon_2(\gamma) - \gamma\epsilon_2'(\gamma)]\rho^2x^2 + \frac{1}{12}\gamma^2\epsilon_2'(\gamma)\rho^3|x|^3 + \cdots, \tag{6}$$

with $x=x_1-x_2$. In the presence of a trapping potential the Tonks parameter becomes space-dependent $\gamma \rightarrow \gamma(x)$. Short-range correlations are expected not to depend on the presence of the confining trap. Figure 3 shows a comparison between g_1 obtained from Eq. (6) and numerical results for different Tonks parameters at the trap center. Taking into account that a high resolution of the short-distance behavior is numerically difficult the agreement is rather good.

The long-range or low-momentum behavior of the correlations can be obtained from a quantum hydrodynamic approach [14] in which long-wave properties of the 1D fluid are described in terms of local-density fluctuations $\delta\rho$ and the phase ϕ: $\hat{\Psi}(x)=\sqrt{\rho(x)}e^{-i\phi(x)}$. The equations of motion for $\delta\rho$ and ϕ follow from the effective Hamiltonian [23,24]

$$H = \int \frac{dx}{2\pi}\{v_N[\pi\delta\rho(x)]^2 + v_J[\partial_x\phi(x)]^2\}. \tag{7}$$

Here $v_N=(\pi)^{-1}\partial\mu/\partial\rho$ and $v_J=\pi\rho$.

In the homogeneous case one finds that the leading-order term in the asymptotics of first-order correlation at temperature T are given by [23]

$$g_1(x_1,x_2) \approx \left(\frac{K/L_T}{\rho\sinh\left(\frac{\pi|x_1-x_2|}{L_T}\right)}\right)^{1/2K}, \tag{8}$$

where $K=\sqrt{v_J/v_N}$ is the so-called Luttinger parameter and L_T is the thermal correlation length $L_T=\pi\rho/KT$, with $k_B=1$. One recognizes that for $T=0$ correlations decay asymptotically as a power law with exponent $1/2K$, while for finite T there is an intermediate power-law behavior turning into an exponential decay for $|x_1-x_2| \gtrsim L_T$. For $T=0$ the exponent $1/2K$ is given by

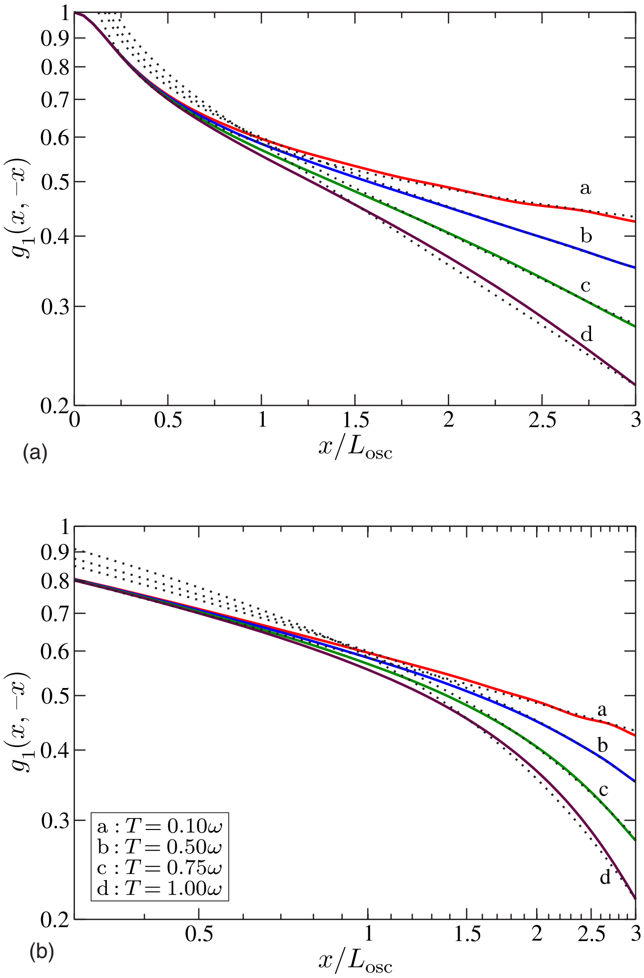

FIG. 4. (Color online) First-order correlations in the temperature regime between exponential and algebraic decay. (a) Semilogarithmic plot. (b) Double logarithmic. Solid curves are DMRG calculations in the trap; dotted lines are harmonic fluid predictions for a homogeneous gas with γ taken at the trap center. Transition from thermal (exponential decay) to quantum-dominated correlations (algebraic decay) at $T \ll \omega$ is apparent. The parameters are $\gamma(0)=3.95$, $N=12$.

$$\frac{1}{2K} = \frac{1}{2}\sqrt{-\frac{\gamma^3 f'(\gamma)}{\pi^2}}. \tag{9}$$

In Fig. 4 we have plotted the first-order coherence $g_1(x,-x)$ for symmetric positions with respect to the trap center for $\gamma=3.95$ and different temperatures. Since for small but nonzero T a much larger number of exited states needs to be taken into account, the number of atoms is practically limited to a few tens. For comparison the harmonic-fluid results for the homogeneous case, Eq. (8), are also shown with K and ρ taken at the trap center and for $T=0$. With the help of the results in Ref. [10] we could determine ρ and K also for $T>0$. However, we find that they do not change significantly in the temperature regime $T<\omega$, so that the difference of decay is mainly coming from L_T. One recognizes two things: First of all the transition from an exponential to a power-law decay happens around $T=0.1\omega$ for which $L_T \approx 30L_{\mathrm{osc}}$. Secondly the correlations are rather well de-

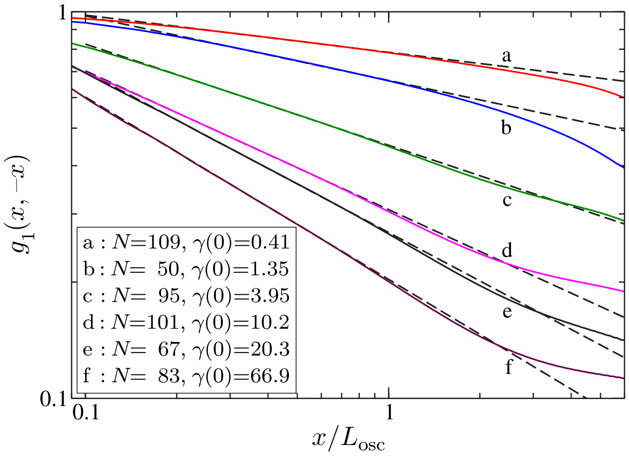

FIG. 5. (Color online) Logarithmic plot of first-order correlations for $T=0$ and various interaction strengths (dots). The dashed lines show power-law prediction from the harmonic-fluid approach with a Luttinger parameter determined by the density at the trap center. γ increases from the top to the bottom curves.

scribed by the homogeneous solution (8). A similar observation can be made at $T=0$. Figure 5 shows the DMRG results for $g_1(x,-x)$ for different interaction strength. The solid lines show the harmonic-fluid predictions for the *homogeneous* case. Again a rather good agreement is found for $x \leq 3L_{\rm osc}$, which on first glance is surprising since the density is space dependent. The agreement is less surprising if one notes that $\gamma(x)$ and thus the local Luttinger parameter $K(x)$ are almost constant within this distance range.

In summary, we have developed a numerical scheme based on the density-matrix renormalization group that allows one to calculate local properties as well as correlations of a 1D Bose gas in a trapping potential for temperatures up to the oscillator frequency. For $T=0$ particle numbers up to 100 can be simulated; for $0<T\leq\omega$ the number drops to a few tens. For local quantities such as the density or the local three-body correlation we found excellent agreement with the predictions from the Lieb-Liniger and Yang-Yang theories with local-density approximation. Deviations from LDA are found only in the immediate vicinity of the edges of the gas or for smaller particle numbers where finite-size effects come into play. We have shown that first-order correlations for positions well within the gas are well described by the homogeneous theory with parameters taken at the trap center. The transition from a thermal-dominated regime of exponential decay to a power-law decay of correlations was shown, with exponents as predicted by the harmonic-fluid approach in the homogeneous case for parameters taken at the trap center.

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