Exact numerical simulations of a one-dimensional, trapped Bose gas

Bernd Schmidt and Michael Fleischhauer
Fachbereich Physik, Technische Universität Kaiserslautern, D-67663 Kaiserslautern, Germany
(Dated: March 23, 2022)

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 and 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.

PACS numbers: 42.50.Gy, 42.25.Bs, 78.0.Ci

Stimulated by the recent experimental progress in generating ultracold trapped quantum gases in one dimension there is a growing interest in correlation properties of these systems. The physics of one-dimensional 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 1D is the transition to the fermion-like Tonks-Girardeau gas for small densities or large interactions. The transition is characterized by a single effective interaction parameter, the Tonks parameter $\gamma$, 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 $T = 0$ and finite $T$. Correlation properties can however not easily be extracted from the Lieb-Liniger solution and require in general numerical techniques such as Monte-Carlo simulations. Approximate analytic expressions can be obtained only for small distances or within the harmonic-fluid approach.

In the presence of a trap potential $V(x)$ integrability is lost. In order to nevertheless calculate local properties Bethe-ansatz solutions for the homogeneous gas can be employed together with a local density approximation (LDA) and the Hellman-Feynman theorem. Recently we have used stochastic simulation techniques to calculate the density profile and first-order correlations of a 1D Bose gas in a harmonic trap. The stochastic simulations were however limited to temperatures larger than the trap energy $k_BT \approx \hbar \omega$ and thus did not allow 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) which leads to results with much higher precision for temperatures form zero to $\hbar \omega$.

We consider a one-dimensional Bose gas with delta interaction in a (harmonic) trapping potential $V(x)$

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

(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 dimension $a_{1D}$.

In the absence of an external trapping potential the Hamiltonian 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 shows that the 1D Bose-gas is fully characterized by one parameter $\gamma = g/\rho$, the so-called Tonks parameter. Here $\rho$ the density of the gas. The Bethe ansatz leads to the so called Lieb equation

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

where $\lambda$ is an implicit function of $\gamma$: $\lambda = \gamma \int_{-1}^{1} dk \sigma(k)$.

All local properties of the gas can be expressed in terms of the (even) moments of $\sigma(k)$

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

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

$$f(\gamma) = \frac{3\epsilon_2(\gamma) \gamma^2 \epsilon(\gamma)}{2\gamma^2}.$$

(2)

Integrability is no longer given when a (harmonic) trapping potential $V(x)$ is taken into account. An often used approximation to nevertheless describe the local properties in the inhomogeneous case is the local density approximation (LDA). The LDA assumes that the homogeneous solution holds with the chemical potential $\mu$ replaced by an effective, local chemical potential.
\[ \mu_{\text{eff}}(x) = \mu - V(x). \]
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:

\[ \rho(x) = \frac{g}{f^{-1}(\frac{\mu_{\text{eff}}(x)}{\gamma})} \]  

where \( f^{-1} \) is the inverse function of eq. [2].

In order to develop an in principle exact numerical algorithm we here want to 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 [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 \( \hat{\Psi}(x) \) by \( \hat{a}_j/\sqrt{\Delta x} \), where \( \hat{a}_j \) is a bosonic annihilation operator. Integrals are replaced by their corresponding sums and the second derivative in the kinetic energy term can be safely approximated by the difference quotient

\[ \frac{\partial^2}{\partial x^2} \hat{\Psi}(x) \approx (\hat{\Psi}(x_{j+1}) + \hat{\Psi}(x_{j-1}) - 2\hat{\Psi}(x_j))/\Delta x^2. \]

This leads to the Bose-Hubbard Hamiltonian

\[ \hat{H} = \sum_i \left[ -J(\hat{a}_i^\dagger \hat{a}_{i-1} + \hat{a}_{i+1}^\dagger \hat{a}_i) + D_i \hat{a}_i^\dagger \hat{a}_i + \frac{U}{2} \hat{a}_i^{\dagger 2} \hat{a}_i^2 \right], \]

where \( J = 1/2\Delta x^2, D_i = 1/\Delta x^2 + V(x_i) - \mu \) and \( U = g/\Delta x \). Expressing the scaled hopping in terms of the Tonks parameter at the trap center, \( J/U = (\gamma \rho(0) \Delta x)^{-1} \) and taking into account that \( a_{1D} \ll \Delta x \ll \rho(0)^{-1} \), the 1D gas corresponds to a compressible phase of the BHM with negative effective chemical potential approaching the line \( \mu_{\text{eff}}/U = -2J/U \). In the limit of vanishing average particle number per site, \( \rho \Delta x \to 0 \), Hamiltonian [11] and [24] become equivalent.

The numerical DMRG calculations of the density profile, shown in Fig. [11], for Tonks parameters \( \gamma \) ranging from 0.4 to about 70 show excellent agreement with the Lieb-Liniger result with LDA [8] apart from a very small region at the edges and the barely visible Friedel-type oscillations, which result from the finite number of particles. 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 \( \gamma \gg 1 \) [24].

An important consequence of the Fermion-like behavior of Bosons in the Tonks limit \( \gamma \gg 1 \) is a dramatic reduction of the loss rate due to inelastic three-body collisions [8]. The rate is proportional to the local three particle correlation \( g_3(x) = \langle \hat{\Psi}^3(x) \hat{\Psi}^3(x) \rangle/\rho(x)^3 \), 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 [22] has found

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

Fig. [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 \( \gamma \) taken at the trap center \( \gamma(0) = g/\rho(0) \). One recognizes again excellent agreement except for a small deviation for very large \( \gamma \), where the numerics is however susceptible to errors due to the smallness of \( g_3 \).

\[ \text{FIG. 1: Density of the 1D bosonic gas in a trap at } T = 0. \] The solid lines are the DMRG results and the dashed lines are the Lieb-Liniger prediction in local density approximation. Increasing values of \( \gamma \) correspond to decreasing densities at the trap center. Insert shows details at the edge of the density distribution.

\[ \text{FIG. 2: Local third-order correlations as function of Tonks parameter at the trap center (red crosses) compared to prediction from Lieb-Liniger theory with local density approximation (solid line) and Tonks-Girardeaux limit (dashed line).} \]
ments 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 Hellmann-Feynman theorem and the asymptotic properties of the Lieb-Liniger wavefunction for large momenta, Olshanii and Dunjko derived the lowest-order terms of the Taylor expansion of \( g_1 \) around \( x_1 - x_2 = 0 \) [13]

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

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

![Figure 3: First order correlations (dashed lines) compared to analytic short-distance expansion (solid lines) for a homogeneous gas with \( \gamma \) taken at the trap center. Values of \( \gamma \) increase from top to bottom curve.](image)

The long-range or low-momentum behavior of the correlations can be obtained from a quantum hydrodynamic approach [14, 15] in which long-wave properties of the 1D fluid are described in terms of two conjugate variables, the local density fluctuations \( \delta \rho \) and the phase \( \phi \): \( \hat{\Psi}(x) = \sqrt{\rho(x)} e^{-i\phi(x)} \). The equations of motion for \( \delta \rho \) and \( \phi \) follow from the effective Hamiltonian [22, 23]

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

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 asymptotic of the first order correlation at temperature \( T \) is given by [22]

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

where \( K = \sqrt{v_J / \rho N} \) is the so-called Luttinger parameter and \( L_T \) is the thermal correlation length \( L_T = \pi \rho / K T \), where we have set \( k_B = 1 \). 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 \( |x_1 - x_2| \geq L_T \). For \( T = 0 \) the exponent \( 1/2K \) is given by

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

![Figure 4: First order correlations in the temperature regime between exponential and algebraic decay. top: semi-logarithmic plot, bottom: double-logarithmic. Solid curves are DMRG calculations in the trap, dashed lines are harmonic fluid predictions for a homogeneous gas with \( \gamma \) 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: \( \gamma = 3.95, N = 12 \). Increasing temperature values correspond to lower curves for large \( x \).](image)
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. For comparison the harmonic-fluid results for the homogeneous case, eq.[3], are also shown with $K$ and $\rho$ taken at the trap center and for $T = 0$. (The change of $K$ and $\rho$ with $T$ has little effect). One recognizes two things: First of all the transition from an exponential to a power-law decay happens around $T = 0.1\omega$. Secondly the correlations are rather well described by the homogeneous solution [3]. A similar observation can be made at $T = 0$. Fig. 5 shows the DMRG results for $g_1(x,-x)$ for different interaction strength. The straight lines show the harmonic fluid predictions for the homogeneous case. Again a rather good agreement is found for $x \leq 3L_{osc}$, which on first glance is rather surprising since the density of the gas is space dependent. The agreement is less surprising if one notes that the local Tonks parameter $\gamma(x)$ and thus the local Luttinger parameter $K(x)$ are almost constant within this distance range. Furthermore replacing $\rho$ in the denominator of eq.[3] by $\rho(x)$ and expanding in a power series one finds that even in the Tonks limit where $K \to 1$ the corrections are small for positions sufficiently far away from the edges of the density distribution.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig5.png}
\caption{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. $\gamma$ increases from top to bottom curves.}
\end{figure}

In summary we have developed a numerical scheme based on the density-matrix renormalization group that allows 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 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. In particular 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.

The financial support through the DFG priority program "Ultracold quantum gases" is gratefully acknowledged.

[1] H. Moritz, T. Stöferle, M. Köhl, and T. Esslinger, Phys. Rev. Lett. 91, 250402 (2003).
[2] T. Stöferle, H. Moritz, Ch. Schori, M. Köhl, and T. Esslinger, Phys. Rev. Lett. 92, 130403 (2004).
[3] B. L. Tolra, K.M. O’Hara, J.H. Huckans, W.D. Phillips, S.L. Rolston, and J.V. Porto, Phys. Rev. Lett. 92, 190401 (2004).
[4] B. Paredes, A. Widera, V. Murg, O. Mandel, S. Fölling, I. Cirac, G.V. Shlyapnikov, T.W. Hänsch, and I. Bloch Nature 429, 277 (2004).
[5] T. Kinoshita, T. Wenger, and D.S. Weiss, Science 305, 1125 (2004).
[6] T. Kinoshita, T. Wenger, and D.S. Weiss, Nature 440, 900 (2006).
[7] L. Tonks, Phys. Rev. 50, 955 (1936).
[8] M. Girardeau, J. Math. Phys. 1, 516 (1960).
[9] E. H. Lieb and W. Liniger, Phys. Rev. 130, 4 (1963).
[10] C.N. Yang and C.P. Yang, J. Math. Phys. 10, 1115 (1969).
[11] V.E. Korepin, N.M. Bogoliubov, and A.G. Izgerin, Quantum Inverse Scattering Method and Correlation Functions (Cambridge Univ. Press, Cambridge, 1993).
[12] G.E. Astrakharchik and S. Giorgini, Phys. Rev. A 68, 031602(R), (2003).
[13] M. Olshanii and V. Dunjko, Phys. Rev. Lett. 91, 090401 (2003).
[14] F.D.M. Haldane, Phys. Rev. Lett. 47, 1840 (1981).
[15] H. Monien, M. Linn, and N. Elstner, Phys. Rev. A 58, R3395 (1998).
[16] K.V. Kheruntsyan, D.M. Gangardt, P.D. Drummond, and G. V. Shlyapnikov, Phys. Rev. Lett. 91, 040403 (2003).
[17] B. Schmidt, L.I. Plimak, and M. Fleischhauer, Phys. Rev. A 71, 041601(R), (2005).
[18] see e.g. U. Schollwöck, Rev. Mod. Phys. 77, 259 (2005), and references therein
[19] C. Kollath, U. Schollwöck, J. van Delft, and W. Zwerger, Phys. Rev. A 69, 031601(R), (2004)
[20] M. Olshanii, Phys. Rev. Lett. 81, 938 (1998); V. Dunjko, V. Lorent, and M. Olshanii, Phys. Rev. Lett. 86, 5413 (2001).
[21] M. A. Cazalilla, cond-mat/0307033 (2003)
[22] M. A. Cazalilla, Phys. Rev. A 67, 053606 (2003).
[23] D.M. Gangardt and G.V. Shlyapnikov, Phys. Rev. Lett. 90, 010401 (2003).
[24] B. Schmidt, L.I. Plimak, and M. Fleischhauer, Phys. Rev. A 71 041601(R) (2005).
[25] V. V. Cheianov, H. Smith, and M. B. Zvonarev, Phys. Rev. A 73, 051604(R) (2006).