Evolution from a Bose-Einstein condensate to a Tonks-Girardeau gas: An exact diagonalization study

Frank Deuretzbacher,[1,*] Kai Bongs,[2] Klaus Sengstock,[2] and Daniela Pfannkuche[1]

[1]*I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstr. 9, 20355 Hamburg, Germany*
[2]*Institut für Laserphysik, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany*

We study ground state properties of spinless, quasi one-dimensional bosons which are confined in a harmonic trap and interact via repulsive delta-potentials. We use the exact diagonalization method to analyze the pair correlation function, as well as the density, the momentum distribution, different contributions to the energy and the population of single-particle orbitals in the whole interaction regime. In particular, we are able to trace the fascinating transition from bosonic to fermi-like behavior in characteristic features of the momentum distribution which is accessible to experiments. Our calculations yield quantitative measures for the interaction strength limiting the mean-field regime on one side and the Tonks-Girardeau regime on the other side of an intermediate regime.

One-dimensional (1D) delta interacting bosons reveal remarkable similarities with non-interacting fermions when the interaction between the particles is strong [1]. The tremendous experimental progress in the field of cold atoms has recently allowed for the realization of such strongly interacting 1D bosonic systems [2–5]. The opposite regime of weak interactions is well described by the Gross-Pitaevskii theory [6,7]. Besides the ground state properties, the dynamical behavior [8] in these two limiting regimes is very different and the excitations follow the Luttinger liquid theory [9,10]. Moreover, an intermediate regime is distinguished [11] by its characteristic phase fluctuations indicating the onset of correlations between the bosons. In the homogeneous thermodynamic limit an exact solution covering all regimes has been introduced by Lieb and Liniger [12], which is the basis of many contemporary approaches [8,13–17]. Correspondingly, most theoretical studies assume large particle numbers. However, gases with strong correlations could only be realized experimentally with a small number of particles so far.

In this article we concentrate on small systems with few particles where the interaction strength between the particles can be tuned by the transverse confinement [5]. In particular, we study the influence of interactions via the pair correlation function which clearly indicates the limits of the mean-field (MF) or Bose-Einstein condensate (BEC) regime, an intermediate regime and the Tonks-Girardeau (TG) regime. The discrimination of these interaction regimes is an important question with relevance for current experiments. We show that the transitions between the BEC, the intermediate and the TG regime can also clearly be distinguished in the evolution of the momentum distribution. The detailed analysis of the correlation function and of the momentum distribution is a central method in the whole field of quantum gases.

We consider spinless bosons (e.g., ^{87}Rb atoms with frozen spin degrees of freedom) confined in a three-dimensional cigar shaped harmonic trap $V_{ext}(\vec{r}) = \frac{1}{2} m \omega_\perp^2 (x^2 + y^2) + \frac{1}{2} m \omega_z^2 z^2$; m is the mass of the bosons, and ω_z and $\omega_\perp$ are the axial and

transverse angular frequencies. The transverse confinement is much stronger than the axial confinement $\omega_z \ll \omega_\perp$. The bosons are assumed to interact via a delta potential $V_{int}(|\vec{r} - \vec{r}'|) = \frac{4\pi\hbar^2 a_s}{m} \delta(\vec{r} - \vec{r}')$, where a_s is the s-wave scattering length.

The system becomes quasi one-dimensional when the transverse level spacing $\hbar\omega_\perp$ is much larger than the axial level spacing $\hbar\omega_z$ and the three-dimensional interaction strength $U_{3D} = \frac{4\pi\hbar^2 a_s}{m l_z l_\perp^2}$ (l_z, $l_\perp$: oscillator lengths of the axial and transverse direction, $l_i = \sqrt{\frac{\hbar}{m\omega_i}}$). Under these conditions the transverse motion in the ground state is restricted to zero-point oscillations. Therefore, the many-particle Hamiltonian reads

$$ H = \hbar\omega_z \sum_i \left(i + \frac{1}{2} \right) a_i^\dagger a_i + \frac{1}{2} U_{1D} \sum_{ijkl} \widetilde{I}_{ijkl} a_i^\dagger a_j^\dagger a_l a_k, \quad (1) $$

where $a_i^\dagger$ (a_i) is the bosonic creation (annihilation) operator for a particle in an energy eigenstate ϕ_i of the axial harmonic oscillator. We have neglected the constant zero mode energy of the transverse oscillator potential. $\widetilde{I}_{ijkl}$ are the dimensionless interaction integrals $\widetilde{I}_{ijkl} = l_z \int_{-\infty}^{\infty} dz \phi_i(z) \phi_j(z) \phi_k(z) \phi_l(z)$. The essential parameter to characterize the system is the one-dimensional interaction strength U_{1D}. It results mainly from an integration over the transverse directions. In addition, the strong vertical confinement leads to a modification of the s-wave scattering length [18]: $a_{eff} = a_s / (1 - 1.46 a_s / \sqrt{2} l_\perp)$. In this paper we restrict ourselves to confining frequencies relevant to the experiments by Kinoshita *et al.* [5], $\omega_\perp = 0 \ldots 2\pi \times 70.7$ kHz, resulting in corrections to a_s of $a_s < a_{eff} < 1.16 a_s$. These values of the transverse frequency are far from the confinement induced resonance discussed in Ref. [18]. Then, $U_{1D} = \frac{U_{3D}}{2\pi} \frac{a_{eff}}{a_s} = 2\sqrt{m\hbar\omega_z} a_{eff} \omega_\perp$, indicating that the effective interparticle interaction can be tuned by the transverse confinement. The Hamiltonian (1) is diagonalized in the subspace of the energetically lowest eigenstates of the non-interacting many-particle system, consisting typically of

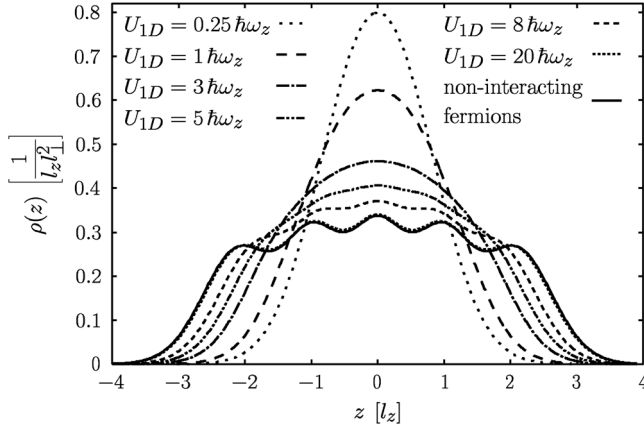*Electronic address: fdeuretz@physnet.uni-hamburg.de

FIG. 1. Particle density of five bosons for different interaction strengths U_{1D} along the axial direction ($x=y=0$). The density becomes flatter and broader with U_{1D}. In the strong interaction regime it develops oscillations. At $U_{1D}=20\hbar\omega_z$ the density of the bosons perfectly agrees with the density of noninteracting fermions.

FIG. 2. Pair correlation function of five bosons for different interaction strengths U_{1D} along the axial direction ($x=y=0$). One particle is fixed at position $z=0$. The distribution flattens and forms a hole at coinciding particle positions, $z=z'$. The correlation function clearly indicates the transition between the three regimes (see text).

up to 150 000 basis states. In the following we will concentrate on results achieved for five bosons.

We start our discussion with the particle density $\rho(z)=\langle\hat{\Psi}^{\dagger}(z)\hat{\Psi}(z)\rangle$ [$\hat{\Psi}(z)$: field operator] which is shown in Fig. 1. At small interaction strength the density reflects the conventional mean-field behavior and $\rho(z)\approx N\phi_{MF}(z)^2$. In this regime all the bosons condense into the same single-particle wave function, $\Psi_B(z_1,\ldots,z_N)\approx\Pi_{i=1}^{N}\phi_{MF}(z_i)$, and thus the many-boson system is well-described by $\phi_{MF}(z)$, which solves the Gross-Pitaevskii equation [6,7]. The system reacts to an increasing repulsive interaction with a density which becomes broader and flatter [13,17,19,20]. In the strong interaction regime density oscillations appear (see, e.g., the curve at $U_{1D}=8\hbar\omega_z$ in Fig. 1) and with further increasing U_{1D} the density of the bosons converges towards the density of five noninteracting fermions, $\rho_F(z)=\Sigma_{i=0}^{4}\phi_i^2(z)$, as predicted by Girardeau [1]. Both densities are in perfect agreement at $U_{1D}=20\hbar\omega_z$ indicating that the limit of infinite interaction is practically reached. Thus, the density oscillations reflect the structure of the occupied orbitals in the harmonic trap. In contrast to Ref. [21] which predicts the oscillations to appear one after the other, when the repulsion between the bosons becomes stronger, we observe a simultaneous formation of five density maxima. These density oscillations are absent in mean-field calculations [13,19].

Additional insight into the evolution of the system with increasing interaction strength can be obtained from the pair correlation function $g^{(2)}(z,z')=\langle\hat{\Psi}^{\dagger}(z)\hat{\Psi}^{\dagger}(z')\hat{\Psi}(z')\hat{\Psi}(z)\rangle$ which is depicted in Fig. 2 for different U_{1D}. In the weak interaction regime where the mean-field approximation is valid the correlation function resembles the particle density and $g^{(2)}(z,z')\approx N(N-1)\phi_{MF}(z)^2\phi_{MF}(z')^2$. The appearance of a minimum at $U_{1D}=0.5\hbar\omega_z$ marks first deviations from this mean-field behavior. The interparticle interaction leads to a reduced probability of finding two bosons at the same position. These correlations are characteristic for the intermediate regime. With increasing interaction strength the correlation hole increases and already at $U_{1D}=3\hbar\omega_z$ the correlation
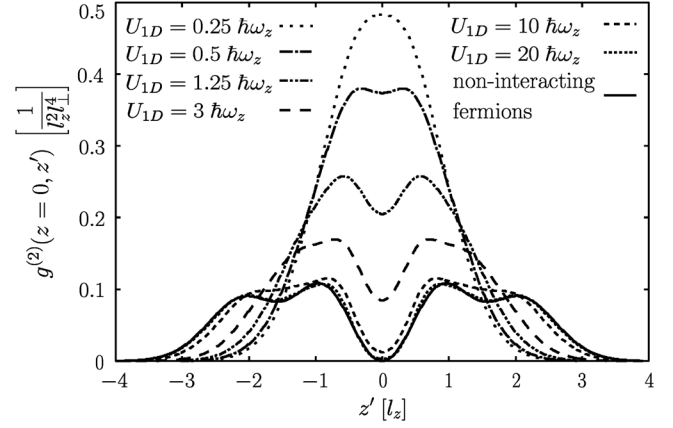
function attains a form which is typical for a Tonks-Girardeau gas: flat long-range shoulders indicate the incompressibility of a Fermi gas. This interaction strength thus marks the transition from the intermediate to the TG regime. By contrast, the density still exhibits a mean-field shape. The correlation function reaches its limiting form corresponding to the one of five non-interacting fermions at $U_{1D}=20\hbar\omega_z$. Besides the central correlation hole maxima appear which indicate the position of the other particles. In our finite size system this limiting behavior is reached at smaller interaction strength than in homogeneous systems [22]. Thus, the pair correlation function clearly indicates the limit of the mean-field regime at small interaction strength ($U_{1D}\lesssim0.5\hbar\omega_z$) and the transition from the intermediate towards the Tonks-Girardeau regime at larger interaction strength ($U_{1D}\gtrsim3\hbar\omega_z$). Within our calculations these limits are not sensitive to the number of particles, which we have checked for up to $N=7$.

We note that, due to the singular shape of the interaction potential, the correlation function exhibits kinks at coinciding particle positions, $z=z'$ [22,24], which are not resolved in Fig. 2 [25]. In recent experiments the correlation function of three-dimensional ultracold atomic systems has been obtained by analyzing the shot noise in absorption images [26,27]. Its value at $z=z'$ [14,15,17] determines, e.g., photo-association rates [28] and the interaction energy. The latter is given by $E_{int}=\frac{U_{1D}}{2}\int dz g^{(2)}(z,z)$ and is depicted in Fig. 3. Its behavior is similar to the homogeneous system due to the short range of the interaction potential [12]. Nevertheless, measurements of the whole pair correlation function are tedious. A quantity which is easier accessible to experiments is the momentum distribution. In the following we demonstrate that the transition between the different regimes discussed above can also be obtained from this quantity.

We first discuss the kinetic energy, $E_{kin,z}=\frac{\langle p_z^2\rangle}{2m}$, which is proportional to the width of the momentum distribution. The limit of the mean-field regime at $U_{1D}\approx0.5\hbar\omega_z$ is clearly vis-
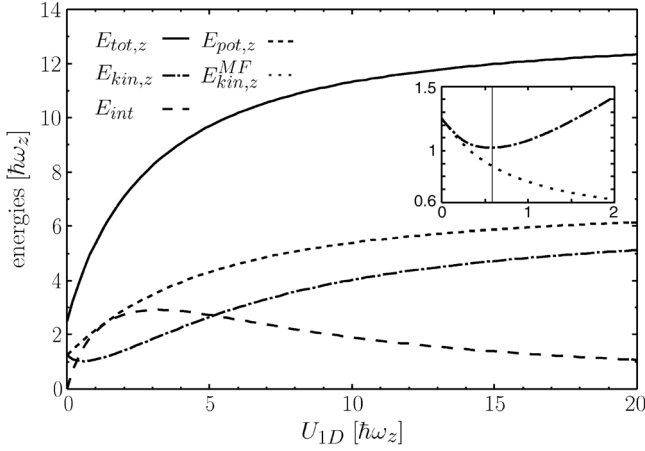
FIG. 3. Evolution of various contributions to the total energy, $E_{tot,z}$, of five bosons with increasing interaction strength U_{1D}. The energies evolve towards the accordant energies of non-interacting fermions [23]. The minimum of the kinetic energy coincides with the onset of significant correlations and therefore marks the limit of the MF regime. By contrast $E_{kin,z}^{MF}$ decreases in the whole interaction regime, see inset.

FIG. 4. Momentum distribution of five bosons for different interaction strengths U_{1D} ($p_x=p_y=0$). The central peak reaches its maximum height at $U_{1D}=3\hbar\omega_z$, see inset. At $U_{1D}=20\hbar\omega_z$ the momentum distribution has developed the typical form of a harmonically trapped TG gas [29] which is completely different from the distribution of noninteracting fermions.

ible in the onset of a minimum of the correlation function (Fig. 2). At the same time the kinetic energy changes dramatically, see Fig. 3. In the weak interaction regime it can be approximated by $E_{kin,z} \approx E_{kin,z}^{MF} = N\frac{\hbar^2}{2m}\int dz[\frac{d\phi_{MF}(z)}{dz}]^2$. The flattening of the density, therefore, results in the initial decrease of the kinetic energy. However, this effect is in competition with the development of short range correlations in the intermediate interaction regime. Strong variations of the wave function at small interparticle distances lead to an increase of the kinetic energy which can be read from the exact expression $E_{kin,z}=N\frac{\hbar^2}{2m}\int dz_1...dz_N[\frac{\partial}{\partial z_1}\Psi_B(z_1...z_N)]^2$. By contrast, the mean-field kinetic energy, which is only sensitive to variations of the density, decreases in the whole interaction regime, see inset of Fig. 3. Therefore, the minimum of the exact kinetic energy clearly marks the limit of the mean-field regime and the dominance of interparticle correlations. With increasing particle number N the minimum of the kinetic energy slightly shifts toward smaller values of U_{1D} with a limit at $U_{1D}=0.5\hbar\omega_z$ at large N.

We mention that the *potential* energy (Fig. 3) is proportional to the width of the particle density, $E_{pot,z}=\frac{1}{2}m\omega_z^2\langle z^2\rangle$. In the strong interaction regime both quantities reach its limiting value of the non-interacting fermionic system. In experiments [5] this has been used as an indication for the Tonks-Girardeau limit.

While the width of the momentum distribution indicates the limit of the mean-field regime the evolution of its central peak marks the transition towards the Tonks-Girardeau regime (Fig. 4). This central result of our studies does not depend on the number of particles. The momentum distribution is defined as $\rho(p_z)=\langle\hat{\Pi}^\dagger(p_z)\hat{\Pi}(p_z)\rangle$ where $\hat{\Pi}(p_z)$ annihilates a boson with momentum p_z. Corresponding to the flattening of the density, the height of the central maximum of the momentum distribution increases at small interaction strength. Already in this regime, high momentum tails de-
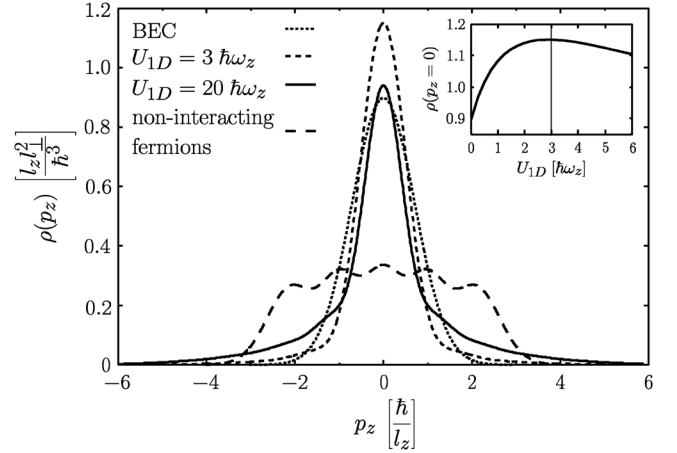
velop due to the kinks in the wave function at coinciding particle positions, $z_i=z_j$ [30,31]. These tails are responsible for the increase of the kinetic energy, i.e., $\langle p_z^2\rangle$, at small interaction strength above $U_{1D}=0.5\hbar\omega_z$. However, the width of the central peak is still shrinking in this regime, corresponding to a further broadening of the density. By contrast, the formation of the correlation hole at $z=z'$ leads to a redistribution from low towards high momentum states. This effect dominates above $U_{1D}=3\hbar\omega_z$, when the growth of the density width slows down. At this point the height of the central peak has reached its maximum. This coincides with the transition behavior visible in the correlation function. Therefore, the interaction strength at which the central peak of the momentum distribution reaches its maximum height marks the
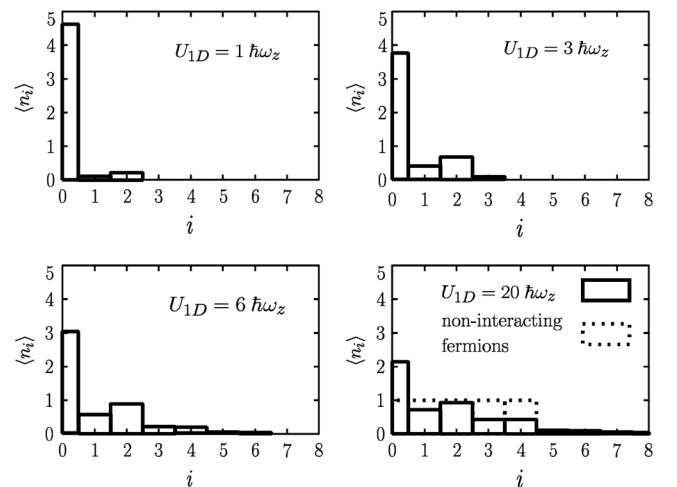

FIG. 5. Occupation number distribution of five bosons for different interaction strengths U_{1D}. With increasing U_{1D} the bosons leave the ground state and occupy excited states. Single-particle states with even parity are comparatively stronger populated than those with odd parity.

transition towards the Tonks-Girardeau regime. Within our calculations the value of $U_{1D}=3\hbar\omega_z$ marking this transition point is independent of the particle number N. The experiments of Tolra *et al.* [3] ($U_{1D}\approx4.91\hbar\omega_z$) and Kinoshita *et al.* [5] (U_{1D} up to $\approx15.4\hbar\omega_z$), therefore, both have been performed in the Tonks-Girardeau regime. The height of the central peak at its maximum is approx. 30% larger than at small interaction strength ($U_{1D}\approx0$) and about 20% larger than at large interactions ($U_{1D}=20\hbar\omega_z$). This contrast increases with increasing particle number. Moreover we mention that the momentum distribution at $U_{1D}=20\hbar\omega_z$ perfectly agrees with exact results obtained in the limit of infinite interaction strength [29].

Finally we discuss the occupation number distribution $\langle n_i\rangle=\langle a_i^\dagger a_i\rangle$ of the 1D harmonic oscillator states which is shown in Fig. 5. With increasing interaction strength U_{1D} the bosons leave the ground state and occupy excited states. At $U_{1D}=20\hbar\omega_z$ the distribution is similar to the distribution shown in [32] for $U_{1D}=\infty$. However, we observe a stronger population of single-particle states with even parity compared to those with odd parity. This effect is most pronounced in mean-field calculations where occupations of odd parity orbitals are absent. The comparatively stronger occupation of single-particle states with even parity can therefore be interpreted as a remnant of the mean-field regime.

In summary, using the exact diagonalization method we studied the interaction-driven evolution of a quasi one-dimensional few boson system. Besides the pair correlation function we identified the momentum distribution as a reliable indicator for transitions of the system between three characteristic regimes, the BEC or mean-field regime, an intermediate regime with strong short-range correlations and the Tonks-Girardeau regime. From this we were able to quantify the interaction strength for the transitions. The width of the momentum distribution has a minimum when the interaction strength is approximately half as large than the axial level spacing of the trap ($U_{1D}=0.5\hbar\omega_z$). This behavior coincides with the onset of significant correlations and therefore marks the transition between the mean-field and an intermediate regime. The central peak of the momentum distribution reaches its maximum height when the interaction strength is approximately three times larger than the axial level spacing ($U_{1D}=3\hbar\omega_z$) and already at this point the pair correlation function attains a form which is typical for a Tonks-Girardeau gas. The evolution of the central peak of the momentum distribution therefore marks the transition between the intermediate and the Tonks-Girardeau regime. These features of the momentum distribution allow a reliable discrimination between the three regimes. We are aware of the limitations of our method to small particle numbers, however, we want to point out that the method of exact diagonalization is capable to reveal the basic microscopic mechanisms of quantum gas systems which often determine the physics of larger systems.

Note added in proof: Recently we became aware of related work by Zöllner *et al.* [33,34].

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[23] The energies shown in Fig. 3 are slightly too large since the complete sweep has been done with a fixed basis set. One can account for the finite basis. From this analysis we get the following true values at $U_{1D}=20\hbar\omega_z$: $E_{tot}=11.78\hbar\omega_z$, $E_{pot}=5.69\hbar\omega_z$, $E_{kin}=5.07\hbar\omega_z$ and $E_{int}=1.02\hbar\omega_z$. The true value of the total energy is 4.6% lower than the total energy shown in Fig. 3. In between, $0\leq U_{1D}<20\hbar\omega_z$, the deviations are smaller.
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the help of the exactly solvable two-boson problem [24].

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