Dynamics of Pair Correlations in the Attractive Lieb-Liniger Gas

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We investigate the dynamics of a one-dimensional Bose gas after a quench from the Tonks-Girardeau regime to the regime of strong attractive interactions applying analytical techniques and numerical simulations. After the quench the system is found to be predominantly in an excited gaslike state, the so-called super-Tonks gas, however with a small coherent admixture of two-particle bound states. Despite its small amplitude, the latter leads to a pronounced oscillation of the local density correlation with a frequency corresponding to the binding energy of the pair. Contributions from bound states with larger particle numbers are found to be negligible.

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Ultracold quantum gases in reduced dimensions have attracted a lot of attention in recent years [1]. This is because on one hand quantum effects play an increasing role in lower dimensions and on the other hand these systems became experimentally accessible using ultracold atomic gases. A striking example is the effective fermionization of a one-dimensional (1D) Bose gas with repulsive interactions, described by the Lieb-Liniger (LL) model [2], leading to the so-called Tonks-Girardeau (TG) gas [3–5]. In the attractive case the ground-state of the LL gas is the highly localized McGuire cluster state [6]. In the thermodynamic limit the gas is unstable, preventing direct experimental studies of ground-state properties. However, in dynamical setups, attractive and repulsive gases are equally well accessible. A recent milestone in this direction is the creation of the super-Tonks-Girardeau (sTG) gas [7,8] by Haller *et al.* [9] realized by a rapid sweep through a confinement resonance from the strongly repulsive to the attractive side. The sTG gas is an excited, gaslike eigenstate, that does not contain any particle clusters. We here analyze the dynamics of this quench process by numerical simulations employing the time evolving block decimation (TEBD) [10,11] algorithm recently applied to the relaxation of the repulsive LL gas [12] and a number of lattice models [13–15].

The Hamiltonian of a 1D, trapped Bose gas with local interactions is given by the LL model [2] with additional potential

$$\hat{H} = \int dx \hat{\Psi}^\dagger(x) \Big[\Big(-\frac{\hbar^2}{2m} \partial_x^2 \Big) + \frac{g}{2} \hat{\Psi}^\dagger(x) \hat{\Psi}(x) + V(x) \Big] \hat{\Psi}(x). \quad (1)$$

g is the interaction strength, which is related to the 1D scattering length a_{1D} via $g = -\hbar^2/(m a_{1D})$, and can have both signs. It is characterized by the dimensionless Tonks parameter $\gamma = 1/(a_{1D}\varrho)$. $V(x) = \frac{m}{2}\omega^2 x^2$ describes a trap.

The spectrum of (1) is quite different depending on the sign of γ; however, the positive- and negative-γ spectra agree in the limits of weak as well as strong interactions [16]. This can be understood from the problem of two particles with $V = 0$ and periodic boundary conditions (PBC): Fig. 1 shows the lowest lying states with vanishing center-of-mass momentum. The noninteracting ground-state (left and right end of the figure at $E = 0$) has a constant relative wave function. For finite interactions, the wave function develops a peak at zero interparticle distance when an attractive interaction ($\gamma < 0$) is turned on and eventually forms a closely bound pair with binding energy $\sim\gamma^2$ (see below). On the repulsive side ($\gamma > 0$) a diplike kink emerges with increasing interaction, which eventually makes the wave function vanish at coinciding particle positions—this is the famous fermionized TG gas. When approaching the strong interaction regime from the attractive side, the first excited state—the sTG gas—adiabatically connects to exactly the same fermionized state. This matching continues for higher excited states and can be generalized to many particles [17].

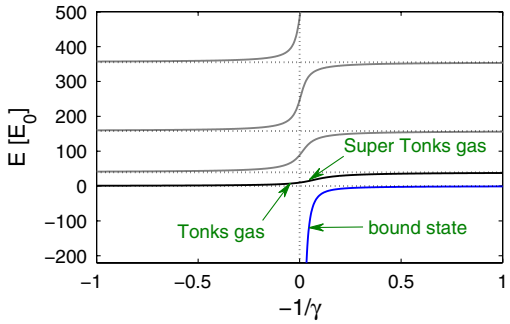

FIG. 1 (color online). Spectrum of LL Hamiltonian for two particles with vanishing total momentum on a ring of length L as a function of inverse interaction strength. The energy unit is $E_0 = 4\pi^2\hbar^2/(L^2 m)$. One recognizes equivalence of the spectra at vanishing ($|\gamma| \to 0$) as well as infinitely strong interactions ($|\gamma| \to \infty$).

Figure 1 indicates that a quench from the TG regime to the strongly attractive regime will put the gas to good approximation in the sTG state. Experiments have successfully demonstrated this, while the difference between TG and sTG can be detected by their different compressibility [7].

We here consider a gas of N particles confined by a harmonic trap initially being in the ground state for $\gamma = +\infty$. At $t = 0$ the interactions are switched to the strongly attractive side $\gamma \ll -1$. In simulations we use values of γ between -6 and -145. The trap plays a minor role, since interactions give the relevant time scale.

We simulate the full many-body dynamics using the numerical TEBD scheme, employing a fourth order trotter decomposition [18]. To this end the continuous model (1) is discretized, resulting in the sparsely filled Bose-Hubbard model [19,20]. The lattice is actually finite, but comprises all of the gas (which does not change its density distribution on the time scale in question). The TEBD algorithm is based on a representation of the state vector in terms of matrix-product states defined on a lattice. In order to be able to perform calculations the dimension of the involved matrices must be kept small corresponding to a small entanglement between different lattice regions. For the specific setup it is necessary that the conservation of the total particle number is taken into account explicitly. While time dependent simulations are generally limited to short times due to the linear growth of entanglement entropy [21,22], this it not crucial here. Although we also observe such a linear growth, the increase is slow and we can go much beyond the time scale of interactions as in [12] for as much as $N = 18$ particles on a 1280 sites lattice using rather small matrices of dimension 100.

Figure 2(a) shows the local two-particle correlation $g^{(2)}(0,0)$, where $g^{(2)}(x_1,x_2) = \langle\hat{\Psi}^\dagger(x_2)\hat{\Psi}^\dagger(x_1)\hat{\Psi}(x_1)\hat{\Psi}(x_2)\rangle/(\varrho(x_1)\varrho(x_2))$, as a function of time for various values of the interaction strength. The correlation function first grows as a power law $\sim(t/t_0)^\alpha$ with a characteristic time $t_0 = 4m/(\hbar\varrho^2)$, which is also used as a time unit in the plots. By a linear fit to the numerical data, we find α growing from 1 in the free case to a value of about $4/3$ in the strongly attractive case. $g^{(2)}$ rises up to a finite value much smaller than 1 for reasonably strong interaction. This reflects the fact that most of the gas ends up in the fermionized sTG state. In addition, we observe a rather peculiar oscillatory behavior with large modulation depth. The frequency coincides with the binding energy of a pair of particles in the McGuire state $\omega_2 \simeq \gamma^2\hbar\varrho^2/4m = \gamma^2/t_0$. Thus the dynamics seems to be strongly affected by the contribution of bound pairs. Moreover, there is no sign of a relaxation, as observed in the repulsive case [12]. In Fig. 2(b) the local three-particle correlation $g^{(3)}$ is plotted. One recognizes that $g^{(3)}$ remains extremely small, showing that higher-order cluster states are not formed. This agrees well with the finding in [23] where the overlap of the TG wave function with the McGuire cluster state was calculated.

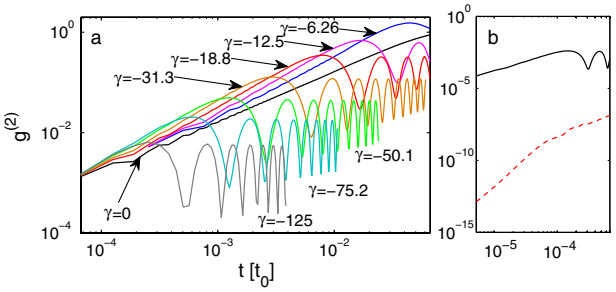

FIG. 2 (color online). Left: Time evolution of the local two-particle density-density correlation in a system of $N = 18$ particles calculated via TEBD (colored lines). Gray line: two-particle case with PBC and $\gamma = 0$. Right: Time evolution of local three-particle correlation $g^{(3)}$ (red dashed) at the trap center and $g^{(2)}$ (black) for comparison at $\gamma = -145$. (The artifacts for very short times are due to the finite time steps used by the numerical algorithm.)

Figure 3 shows the dynamical evolution of the density-density correlations, where we fix one position at the center of the cloud. The initial state shows the typical feature of fermionization; i.e., $g^{(2)}(0,0)$ is zero and $g^{(2)}(0,x)$ rises to one (no correlation) on a length scale proportional to the average interparticle distance. In the limit $\gamma \to -\infty$ the correlations do not show much resolvable dynamics because the initial TG is close to the sTG state. However, for moderate interaction strength, we see $g^{(2)}(0,x)$ rising sharply around zero distance. This clearly shows transitions to states other than the sTG state. One finds that the characteristic length scale of the peak at the origin is given by a_{1D}. This gives further indication of a finite admixture of the $N = 2$ cluster state. Note, that since $\int dx\langle\hat{\Psi}^\dagger(x)\hat{\Psi}^\dagger(0)\hat{\Psi}(0)\hat{\Psi}(x)\rangle = \varrho(0)(N-1)$ the integral over $g^{(2)}(0,x)$ must be constant in time, as long as the density is homogeneous. The increase at $x_1 - x_2 = 0$

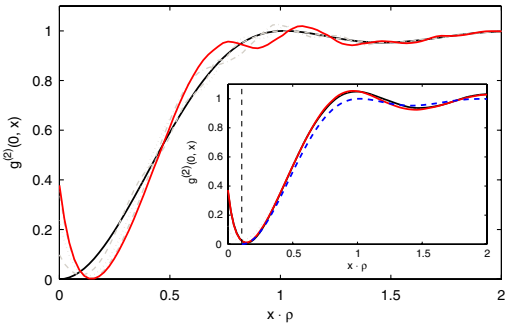

FIG. 3 (color online). Time evolution of the nonlocal density-density correlation function for interaction strength $\gamma = -18.7931$ calculated for $N = 18$ particles using TEBD. Curves are shown for 0 (black), 1/4 (dotted), and 1/2 (red, maximum value at $x = 0$) oscillation periods of the local correlation. Inset: $g^{(2)}$ at times of 3.5 (black, solid), 4 (dotted), and 4.5 (red, maximum value at $x = 0$) periods. The vertical dashed line indicates $x = a_{1D}$. The blue dashed line shows $g^{(2)}$ for a TG gas shifted by a_{1D} and renormalized.

must therefore be accompanied by a decrease at larger distances as seen in the correlation waves building up in Fig. 3. The inset of Fig. 3 shows another interesting feature: apart from small distances, where oscillations continue, the correlations become quickly stationary (at least over several oscillation periods) and can be well approximated for intermediate distances by $g^{(2)}$ of a TG gas shifted by a_{1D} and renormalized by a factor $(1-\gamma^{-1})$ (dashed, blue line). This can be explained as follows: As shown in [23] the wave function of the two-particle problem with finite attractive interactions has a node at some distance $x=a$ and for larger distances coincides with the TG wave function apart from normalization. For large $|\gamma|$, $a \approx a_{1D}$. Furthermore, the renormalized and shifted TG correlation curve agrees very well with $g^{(2)}(0,x)$ for a system of hard rods with excluded volume $a \approx a_{1D}$ [24]. The fact that the TEBD results show slightly more pronounced oscillations than the shifted TG or hard-rod curve is due to the small excitation of higher gaslike states.

We will show now that the two-particle correlations in the trapped gas can be very well reproduced by a system containing only $N=2$ particles. This is due to the fact that eigenstates are expected to be well approximated by pair product states of the Jastrow-Bijl type [23]

$$\Phi(x_1,\ldots,x_n)=\Big[\prod_{i<j}\varphi(x_i-x_j)\Big]\prod_{j=1}^{N}\exp\Big(-\frac{x_j^2}{2l_{\mathrm{osc}}^2}\Big), \quad (2)$$

with $l_{\mathrm{osc}}^2=\hbar/(m\omega)$, and $\varphi(x_i-x_j)$ being a two-particle wave function. The two-particle solution will provide insight into the nature and the size of the oscillations observed in the numerics. For the actual calculations we impose PBC, which is reasonable for the comparison to the trapped gas, since the latter is homogeneous to good approximation over some interparticle distances. The PBC problem gives analytical expressions and allows us to extract the scaling with γ in the strongly interacting regime. This problem has been solved in the original paper by Lieb and Liniger [2], and we will use their solution.

The Hamiltonian for the two-particle problem reads in first quantization $\hat{H}=-\frac{\hbar^2}{2m}(\partial_1^2+\partial_2^2)+g\delta(x_1-x_2)$. All eigenstates can be constructed from coordinate Bethe ansatz [25]. In the primary sector $(0\le x_1\le x_2\le L)$, the solution is $\varphi(y=x_1-x_2)=2Ae^{i(\delta/4)}\cos[\frac{\delta}{2}(\frac{y}{L}-\frac{1}{2})]$. A is a normalization constant, and δ is related to the scattering phase shift $\Theta=-2\tan^{-1}[(k_2-k_1)L/2\gamma]$ via $\Theta=\delta/2-\pi$. Note that $e^{i(\delta/4)}$ is not a simple phase factor as δ will be imaginary for the bound state.

We will now calculate asymptotic expressions for the bound state φ_b, where $\gamma\to-\infty$, as well as TG and sTG states $\varphi_\pm$, where $\gamma\to\pm\infty$. For the bound state φ_b we need to find an imaginary solution of the Bethe equation. Substituting $\delta=i\tilde{\delta}$ we find in the strongly interacting limit $\tilde{\delta}=(-2\gamma)$. With this we calculate the normalization of the wave function, yielding $A_b\to\sqrt{\tilde{\delta}/2}/L$. Thus

$$\varphi_b(x_1-x_2=0)=2A_be^{-(\tilde{\delta}/4)}\cosh\frac{\tilde{\delta}}{4}\overset{\gamma\to-\infty}{\longrightarrow}-\frac{\sqrt{-\gamma}}{L}. \quad (3)$$

Because of bosonic statistics the local two-particle correlation is given in terms of the wave function as $g^{(2)}(0,0)=2|\varphi(0)|^2/\varrho(0)^2$. As the density ϱ is $2/L$ everywhere, this results in $g_b^{(2)}(0,0)\to\tilde{\delta}/4=-\gamma/2$.

We denote the lowest lying gaslike states $\varphi_\pm$ for $\gamma\to\pm\infty$. From the Bethe equation we see that a real solution δ will be close to 2π. Expanding the tangent around its singularity at $\pi/2$ we get $\delta=2\pi(1-\frac{2}{\gamma})$. For the normalization this means $A_\pm\to 1/L\sqrt{2}$, such that

$$\varphi_\pm(x_1-x_2=0)=2A_\pm e^{(i\delta/4)}\cos\frac{\delta}{4}\overset{\gamma\to-\infty}{\longrightarrow}i\sqrt{2}\frac{\pi}{\gamma L}. \quad (4)$$

The local two-particle correlation is in this case $g_\pm^{(2)}(0,0)=\pi^2/\gamma^2$. The γ^{-2} scaling is well known [26] and is the same as in the many-particle case.

The overlap between the initial TG gas $\varphi_0=\lim_{\gamma\to\infty}\varphi_+$ and the bound state can easily be calculated for large $|\gamma|$. One finds $\epsilon\equiv\langle\varphi_0|\varphi_b\rangle\to-2\sqrt{2}\pi\gamma^{-3/2}$.

We now want to calculate the dynamics of the local correlation in the two-particle case. This can be done in many different ways. We used discretization [12] and exact diagonalization to find the solution shown in Fig. 4 as a black solid curve. From the above calculations we can derive simple approximations which are very good in the strongly interacting regime. We can decompose the initial state $|\varphi_0\rangle$ according to

$$|\varphi_0\rangle=\epsilon|\varphi_b\rangle+(|\varphi_0\rangle-\epsilon|\varphi_b\rangle)=\epsilon|\varphi_b\rangle+|\bar{\varphi}_0\rangle. \quad (5)$$

Note that for large $|\gamma|$, $|\bar{\varphi}_0\rangle$ is approximately normalized. Since the initial state is the TG gas with $\varphi_0(x_1-x_2=0)=0$ one finds from (5) and (3) for $t=0$:

$$\bar{\varphi}_0(x_1-x_2=0,t=0)\overset{\gamma\to-\infty}{\longrightarrow}i2\sqrt{2}\frac{\pi}{\gamma L}. \quad (6)$$

Note the factor of 2 as compared to Eq. (4) which is physically due to the very small admixture of the bound

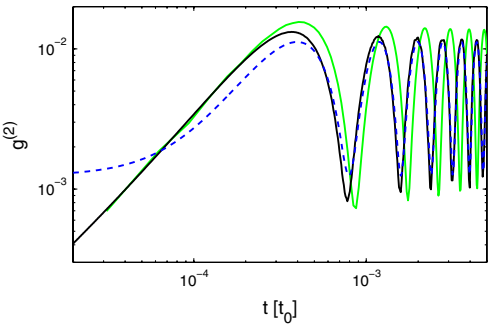

FIG. 4 (color online). Comparison of the many-body results with the results from the two-particle system with PBC in the case $\gamma=-89.0355$. The thick black line corresponds to the two-particle case, the thin green one shows the $N=9$ particle case (calculated via TEBD), and the blue dashed one is the beating approximation (8).

state. $\bar{\varphi}_0$ is not an eigenstate, but is composed of low-lying gaslike states, that have an energy spread much smaller than the pair binding energy. For small times one can ignore the energy differences and thus the time dependence of $\bar{\varphi}_0$. This results in

$$g^{(2)}(t) \overset{\gamma\to-\infty}{\longrightarrow} 8\frac{\pi^2}{\gamma^2}[1-\cos(\omega_2 t)]. \quad (7)$$

This expression describes the initial increase of $g^{(2)}$ as observed in the many-particle calculation (and in the numerical solution of the $N=2$ case) very well. It does predict, however, oscillations with unity modulation depth, which is not true. The reason for this is that $\bar{\varphi}_0$ contains in addition to the dominant, lowest gaslike state (i.e., the sTG state) φ_- also small admixtures of higher lying gas states which oscillate in time all with slightly different frequencies. For larger times these oscillations lead to an effective dephasing in the interference part of $g^{(2)}$. Note that the direct contribution of the excited gas states to $g^{(2)}$ is negligible. An approximation which is much better suited to describe the large time behavior is $|\varphi_0\rangle \approx \epsilon|\varphi_b\rangle + |\varphi_-\rangle$. Comparing (4) and (6) shows, that we have only changed a factor of 2 such that

$$g^{(2)}(t) \overset{\gamma\to-\infty}{\longrightarrow} \{5-4\cos[(\omega_2+\pi^2/t_0)t]\}\frac{\pi^2}{\gamma^2}, \quad (8)$$

where we used that the sTG gas energy is $\hbar\pi^2/t_0$ for strong interaction, giving a minor correction to the frequency. On short time scales this expression is invalid, but for $t > t_0/\gamma^2$ it becomes a much better approximation than (7), as shown in Fig. 4. It is interesting to note that $g^{(2)}$ scales as $1/\gamma^2$, while the pair fraction, i.e., the probability to find particles in a paired state, $\eta = |\varepsilon|^2 = 8\pi^2/|\gamma|^3$ scales as $|\gamma|^{-3}$ and is thus more difficult to observe for large $|\gamma|$.

In summary, we have shown by numerical TEBD simulations that an interaction quench of a 1D Bose gas from strong repulsive to strong attractive interactions puts the gas predominantly into the lowest gaslike state, the sTG gas. There is, however, a small coherent admixture of two-particle bound states that results in a large-amplitude oscillation of the local density correlation with a frequency corresponding to the energy difference between sTG gas and bound pair state. At the same time higher-order correlations remain extremely small showing that more deeply bound, multiparticle cluster states are not formed. Analytical calculations of the $N=2$ case were found to reproduce the many-particle results with high accuracy. This indicates that the many-body state can be well approximated by a Jastrow-Bijl type pair product wave function, where each term is a coherent superposition of a gaslike state with a very small component of a two-particle bound state. The peculiar oscillations of $g^{(2)}$ show furthermore that despite their small weight, the two-particle cluster states are accessible to experimental probes. For strong interactions, the bound pairs are highly colocalized. Since in all physical realizations of the LL model, the true interparticle potential is of finite range, details of the potential will show up in the binding energy. In this way, the two-particle correlation dynamics can be used to measure details of the underlying true potential. In order to assess whether the effect predicted is accessible in current experiments let us compare the beat frequency $\omega_2 = \gamma^2\hbar\varrho^2/4m$ to the transverse trap frequency $\omega_\perp$. Introducing the longitudinal trap frequency $\omega_\parallel$ one finds $\omega_2 = \gamma^2 N\omega_\parallel/4$. For $\gamma \approx 10$ and 10 particles per tube this gives $\omega_2 \approx 250\omega_\parallel$. For the experiment of [9] this corresponds to about 3 kHz which is only a factor of 4 smaller than $\omega_\perp$. Using larger laser beam diameters this factor can be increased, however, to 1 order of magnitude, such that the 1D approximation remains valid [27]. Furthermore, our numerics showed that the oscillations with a single dominant frequency ω_2 prevail even for values of γ as low as -1, which would result in a reduction of ω_2 by 2 orders of magnitude. Finally, our Letter shows that the TEBD algorithm is suitable for the simulation of dynamical processes in strongly interacting, continuous quantum gases.

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