Metastable Criticality and the Super Tonks-Girardeau Gas

Milosz Panfil,* Jacopo De Nardis, and Jean-Sébastien Caux
Institute for Theoretical Physics, University of Amsterdam, Science Park 904, Postbus 94485, 1090 GL Amsterdam, The Netherlands

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We consider a 1D Bose gas with attractive interactions in a highly excited state containing no bound states. We show that in this so-called super Tonks-Girardeau gas, relaxation processes are suppressed, making the system metastable over long time scales. We compute dynamical correlation functions, revealing the structure of excitations, an enhancement of umklapp correlations and new branches due to intermediate bound states. These features give a clear signature of the super Tonks-Girardeau regime and can be used to experimentally identify it. We demonstrate that, despite its off-equilibrium nature, the system displays critical behavior: correlation functions are characterized by asymptotic power-law decay described by the Luttinger liquid framework.

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Quantum many-body systems exhibiting strong correlations are of prime interest from both theoretical and experimental perspectives: they witness the breakdown of the simple single-particle excitation picture, opening up new possibilities for interesting states and excitations. In one dimension, interactions generally lead to fractionalized low-energy collective modes displaying quantum critical behavior [1]. One prominent example is the 1D Bose gas [2,3], which can be, by now, experimentally realized and probed in and out of equilibrium [4–7] with tunable interaction strength [8].

An interesting set of questions is: how strong can correlations become, and how do they reshape physical properties? It is well known that infinitely strong repulsive pointlike interactions (giving the Tonks-Girardeau gas [9,10]) lead to effective fermionization of the degree of freedom. One way to make correlations stronger is to consider longer-ranged interactions, as in a dipolar gas [11]. On the other hand, turning on attractive interactions has an even more dramatic effect of leading to the formation of bound-state quasiparticles. The ground state then becomes a macroscopic bound cluster [12], with strongly gapped dynamical responses [13].

An interesting alternative for the attractive 1D Bose gas is to consider a highly excited state in which no bound states are present, all particles being in a low-lying gaseous state. This system was subjected to recent experimental [6] and theoretical [14–19] studies, and is known as the super Tonks-Girardeau gas (sTG). Contrary to the ground state of the attractive gas, this state displays a finite energy per particle in the thermodynamic limit. The structure of its excitations is similar to that found in fermionic systems, with the addition of bound states. It is our purpose in this Letter to perform a theoretical analysis, using an integrability-based method, of the dynamical responses of the sTG gas. Our aim is to highlight its experimentally observable features, facilitating its identification in the laboratory. Interestingly, correlations in this off-equilibrium state still display quantum-critical Luttinger liquid universality-class behavior, as will be clear from our results.

The Letter is organized as follows. After introducing the system and the correlations we intend to study, we describe its excitations in detail, focusing on those relevant to the sTG state. After discussing the stability of this state and showing that its decay rates are sufficiently small to make it metastable on realistic time scales, we compute its density-density correlations in momentum space and real space. We end with a discussion of the system’s quantum critical features.

Setup.—Our starting point is the Lieb-Liniger Hamiltonian (taking \( h = 2m = 1 \)) [2] for \( N \)-particles in a cyclic system of length \( L \),

\[
H_{LL} = -\sum_{i=1}^{N} \partial_{x_i}^2 + 2c \sum_{i<j}^{N} \delta(x_i - x_j), \tag{1}
\]

where \( c \) parametrizes interactions, which we take to lie in the attractive regime \( (c < 0) \). We address correlations by studying the density-density function defined by its Lehmann representation

\[
S(k, \omega) = \frac{2\pi}{L} \sum_{\lambda \in \mathcal{H}} |\langle \lambda | \rho_{\lambda} | sTG \rangle|^2 \delta(\omega - E_{\lambda} + E_{sTG}), \tag{2}
\]

where \( \lambda \) labels eigenstate with energy \( E_{\lambda} \) in the Hilbert space \( \mathcal{H} \), and \( \rho_{\lambda} \) is the Fourier transform of the density operator \( \rho_{\lambda} = \sum_{q} \Psi_{q+}^\dagger \Psi_{q} \) (where the operators \( \Psi_{q}^+, \Psi_{q} \) satisfy canonical bosonic commutation relations \( [\Psi_{q}, \Psi_{q'}^+] = \delta_{q,q'} \)). We denote with \( | sTG \rangle \) the sTG state; its explicit definition will be provided after we discuss the eigenstates. The density-density correlation is experimentally accessible with Bragg spectroscopy [20].
The Lieb-Liniger Hamiltonian (1) is exactly solvable by Bethe ansatz [2]. The $N$-particle wave function is given by a linear combination of plane waves

$$
\Psi(x_1, \ldots, x_N) = \prod_{j<k}^{N} \sgn(x_j - x_k) \sum_{P} A_P e^{iL \sum_{j=1}^{N} \lambda_j x_j} \tag{3}
$$

with $A_P = (-1)^{\mu} e^{i\sum_{j<k} \sgn(x_j - x_k) \phi(\lambda_j - \lambda_k)}$ and the two-particle phase shift $\phi(\lambda) = 2 \arctan(\lambda/c)$. By imposing periodic boundary conditions, rapidities $\{\lambda_j\}_{j=1}^{N}$ get quantized via the Bethe equations

$$
\lambda_j + \frac{1}{L} \sum_{k=1}^{N} \phi(\lambda_j - \lambda_k) = \frac{2\pi}{L} I_j. \tag{4}
$$

The quantum numbers $\{I_j\}_{j=1}^{N}$ are integers ($N$-odd) or half-odd integers ($N$-even) and completely specify the eigenstate. The Hilbert space of $H_{1L}$ is spanned by different choices of sets $\{I_j\}$. The momentum of the eigenstate is $P_\lambda = \sum_{j=1}^{N} \lambda_j$, whereas the energy equals $E_\lambda = \sum_{j=1}^{N} A_j^2$.

The structure of the Hilbert space is different depending on the sign of interactions. Characteristic for repulsive interactions is a Pauli-like principle: quantum numbers must be mutually distinct and all solutions to the Bethe equations are real. Attractive interactions drastically change this by allowing complex rapidity solutions [12]. These then form regular patterns in the complex plane (strings) with exponentially small corrections in the system size, which for the system size considered here are completely negligible. Strings are symmetric around the real axis, their imaginary parts having a spacing of $|c|$. They are naturally understood as bound states representing independent, stable particles. The nonzero imaginary part of rapidities causes exponential decay of the wave function for increasing separation of two particles within a string, with a characteristic distance $|c|^{-1}$ [12].

The ground state is formed by a single bound state ($N$-string). All other eigenstates can be constructed by two basic operations, either by breaking them and/or by giving them momentum. In the attractive regime, the Pauli principle holds between strings of the same length. The state classification is then straightforward.

$sTG$ gas.—For a system with $N$-particles, we explicitly define the $sTG$ state as a collection of one-strings with the following choice of quantum numbers:

$$
I_j^{sTG} = -\frac{N+1}{2} + j, \quad j = 1, \ldots, N. \tag{5}
$$

The $sTG$ state is thus the lowest-lying, purely gaslike state with no bound states; it has a Fermi sea structure similar to the ground state of the repulsive gas (Fig. 1); this fact ultimately explains its quantum critical behavior, to be seen later in the correlations we compute.

Such a state can be experimentally realized by employing a confinement-induced resonance [6,8]. Quenching the magnetic field over the resonance changes the sign of the interactions. Starting in the ground state of the TG gas, the interaction parameter is quenched to the other side of the resonance. Quenching to $c = -\infty$ exclusively populates the $sTG$ state. Quenching to a finite but large negative value of $c$ leads to a combination of states with the $sTG$ state being predominant, all other states having an amplitude suppressed by at least a factor $|c|^{-2}$. In fact, observing the correlation features which we give below, would allow one to quantify the “closeness” to the $sTG$ state obtained in an actual experiment.

In order to compute correlations we first need to classify the excitations around the $sTG$ gas. One class of excitations are the particle-hole excitations paralleling those of the repulsive gas [2]. We can again distinguish type I and type II modes, which can be combined to create multiparticle-hole excited states (see Fig. 1(b)). These excitations lead to a modified version of correlations as compared to the repulsive gas; attractive interactions inducing smooth changes to the particle-hole contribution to the correlation as one tunes $1/c$ through zero.

Other classes of excitations involve bound states of two or more atoms [see Fig. 1(c)]. These lead to new branches of correlations, which we discuss in the next section. The gas is ultimately metastable due to particles progressively binding into such energetically favorable kinds of excitations. However, as we show here, the rate of formation of bound states induced by generic perturbations is small. The estimate of this rate confirms that the system is sufficiently long-lived to be experimentally observable.

We examine the simplest (and most probable) process: the formation of a two-string (bound state with two particles) in order to quantify the time scale for stability of the gas. Consider adding a localized impurity potential $\tilde{V} = \alpha \epsilon_F n_{1D}(x = 0)$ to the otherwise isolated system. Here $\alpha$ is a dimensionless constant, $\epsilon_F = (\hbar \pi n_{1D})^2/2m$ is the Fermi energy, $n_{1D}$ is the 1D density, and $m$ is the atomic mass. Such a perturbation induces decays whose rate can be computed using Fermi’s golden rule. Assuming that the external potential is weak (we set
\( \alpha = 0.1 \) for a gas of \(^{133}\text{Cs}\) atoms of 1D density \( n_{1D} = 10^6 \text{ m}^{-1} \) with \( c/n_{1D} = -8 \), we get a rate \( \Gamma_{2-\text{str}} = (\alpha \epsilon_F / h n_{1D})^2 S(\omega = 0^-) \sim 1 \text{ s}^{-1} \). \( S(\omega = 0^-) \) is the density-density correlator summed over all momenta [see Eq. (7)] and taken at the slightly negative value of the energy so that only bound states contribute. For larger attractive interactions and weaker perturbations the time scale is much larger. A typical experimental time scale is \( -10^{-3} \text{ s} \) and is thus shorter than \( \Gamma_{2-\text{str}} \). For repulsive interactions the stability of the gas is controlled by the rate of 3-body collision [21]; as this rate is of the same order as \( \Gamma_{2-\text{str}} \), the sTG gas can be viewed in practice as being as stable as the repulsive gas.

A physical picture of this stability is as follows: for a two-string to form, two particles must be a distance \( |c|^{-1} \) apart. This is, however, highly unlikely since the initial nonlocal pair correlation function [\( S(x) \)] exhibits fermionic behavior; at small distances its value is small. This shows that decay channels are not really open (for \( c = -\infty \) they are, in fact, completely closed since the rates from Fermi’s golden rule vanish). We analyze the behavior of \( S(x) \) in the next section. Further evidence for the stability of the sTG gas is provided by numerical computation of the compressibility of the gas, which is positive for large attractive interactions [14].

### Density-density correlation function

We directly compute the Fourier transform of the density-density correlation function [\( S(k) \)] by adapting the method used previously for the repulsive gas [22]. The matrix elements of the density operator (form factors) are known exactly through the methods of algebraic Bethe ansatz [23]. Equation (2) demonstrates the computational method. The ABACUS algorithm [24] was used to recursively explore the Hilbert space looking for states that contribute the most to the correlation. We obtained highly accurate results for the density-density correlation function for \( N = 128 \), the \( f \)-sum rule identity \( \int_{-\infty}^{\infty} \omega S(k, \omega) d\omega = \frac{\pi k^2}{L} \) giving a quantitative check (Table I).

### Momentum space

The dynamical correlation is plotted in Fig. 2. As the sTG state takes the form of a Fermi sea, its low-lying type I and II excitations have a linear spectrum and this sector of the sTG gas falls into the Luttinger liquid universality class, with Luttinger parameter \( 0.5 < K < 1 \) (see inset of Fig. 3). The behavior of the correlation along the edges of support of a single particle-hole excitation agrees, in fact, with the predictions of nonlinear Luttinger theory [25]. For values of \( K > 1 \) (repulsive interactions) there is a singularity along the type I mode (upper threshold) and smooth vanishing of correlation along the type II mode (lower threshold). For \( 0.5 < K < 1 \), inversely, the correlation is smooth along the particle mode and diverges along the hole mode. This shift of correlation weight towards the lower threshold is clearly seen in our data (see Figs. 2 and 3). Additionally, bound states contribute in another window of energies starting below zero (because of the binding energy of a two-string). Since the correlation weight carried by those states vanishes for infinite \( |c| \), the most interesting situation occurs when the interaction is not too large: one then sees a new, broad branch of correlations developing around a dispersing bound state (see Fig. 2, bottom).

Two other interesting quantities, namely, the static correlator and the dynamical autocorrelator

\[
S(k) = \int_{-\infty}^{\infty} S(k, \omega) \frac{d\omega}{2\pi},
\]

\[
S(\omega) = \frac{1}{L} \sum_k S(k, \omega),
\]

are plotted in Fig. 4. The shift of the correlation weight towards the lower threshold leaves a characteristic mark in the static correlator [Eq. (6) and Fig. 4] [14]. For repulsive interactions, the static correlator around \( k = 2k_F \) smoothly approaches its asymptotic value from below [\( S(k) \to 1 \)]. Here at \( k = 2k_F \) we observe a divergence of the correlator and a power-law tail above the asymptote.

FIG. 2 (color online). The density-density correlation in momentum and energy space for \( c = -8 \), \( c = -16 \), and \( c = -64 \). The negative energy parts of the plots were rescaled by factors 10, 100, and \( 2.5 \times 10^5 \), respectively, to make the string contribution easier to see. The discontinuity in the \( c = -8 \) plot around \( \omega = 0 \) is an artifact of this rescaling. As the interactions become more attractive, the correlation weight spreads uniformly between the lower- and upper-thresholds of the single particle-hole continuum, just as for the TG gas. At the same time, the contribution from intermediate bound states is suppressed in value and moves to lower energy.

### Table I

Levels of saturation of the \( f \)-sum rule. All computations were performed at unit filling (\( N/L = 1 \)) and for \( N = 128 \) particles.

<table>
<thead>
<tr>
<th>( c )</th>
<th>( k = k_F )</th>
<th>( k = 2k_F )</th>
<th>( k = 3k_F )</th>
<th>( k = 4k_F )</th>
</tr>
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<tbody>
<tr>
<td>( c = -8 )</td>
<td>99.7%</td>
<td>99.7%</td>
<td>99.9%</td>
<td>99.9%</td>
</tr>
<tr>
<td>( c = -16 )</td>
<td>99.3%</td>
<td>99.3%</td>
<td>99.9%</td>
<td>99.9%</td>
</tr>
<tr>
<td>( c = -64 )</td>
<td>99.9%</td>
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</tr>
<tr>
<td>( c = -256 )</td>
<td>99.9%</td>
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Moreover, for less attractive interactions, the dynamical autocorrelator \( S(\omega) \) [Eq. (7) and Fig. 4] develops a plateau on the negative side of \( \omega \). This plateau is a clear signature of the attractive gas and of contributions coming from intermediate bound states. Together with the divergence at the lower threshold, these are the two smoking guns to look for experimentally.

**Real space.**—We now move on to real space and inspect the Fourier transform of the static correlator

\[
S(x) = \frac{1}{L} \sum_k e^{-ikx} S(k).
\] (8)

From the behavior of \( S(x) \) for small \( x \) we can infer the effective statistics of the particles (Fig. 5). We see the fermioniclike behavior, which is robust to changes in the interaction [19]. This is similar to the fermionization process in the repulsive 1D Bose gas [10].

At large distances, results can be compared with Luttinger liquid theory, which predicts [1,26] the large distance asymptote of correlations as a series,

\[
S_{LL}(x) = 1 - \frac{K}{2(\pi x)^2} + \sum_{m=1} A_m \cos(2mk_Fx) x^{-2mK}. \] (9)

In the sTG case, this formula describes the leading particle-hole contributions to the correlations. The prefactors \( A_m \) in Eq. (9) are not universal. They depend on the microscopic theory and are connected with the scaling limit of form factors [27]. This, in turn, allows for the exact computation of prefactors in integrable theories where form factors are explicitly known. Figure 5 depicts the comparison between the correlations computed for \( N = 128 \) and the asymptotics (including prefactors) from Ref. [27]. The accurate match is yet another illustration of the applicability of the theory of Luttinger liquids in this off-equilibrium context.
Conclusions and outlook.— In this Letter we considered the super Tonks-Girardeau gas and its correlations. We showed that attractive interactions drastically modify the dynamical responses of the system, while leaving it metastable over long time scales. The system exhibits even stronger collective behavior than its repulsive counterpart, with the majority of the density-density correlation carried by the type II mode and an enhancement of umklapp correlations around $2k_F$, ultimately causing the divergence of the static correlator at $k = 2k_F$. On top of this, there are intermediate bound states with an extended region of correlation for $\omega < 0$. In experimental realizations, observing these features would allow one to confirm that one has, indeed, constructed a clean version of the super Tonks-Girardeau gas.

We also showed that, despite attractive interactions and metastability, the super Tonks-Girardeau gas, due to its structure still resembling a closed Fermi sea, still displays the standard features of a quantum critical liquid. The system has a sector of excitations which falls into the Luttinger liquid universality class, whose contributions set the leading long-distance asymptotes of correlations in agreement with Luttinger liquid theory. The subleading contributions coming from bound states could be reintroduced by treating them as mobile quantum impurities, in a similar fashion to the case of spin impurities in ferromagnetic Luttinger liquids [28]. Going further, initial metastable quantum-critical states similar in spirit to the sTG state can exist in other systems (e.g., multicomponent bosons, fermionic Luttinger liquids [28]). We will investigate these issues in future publications.

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* m.k.panfil@uva.nl