Equilibration of a Tonks-Girardeau Gas Following a Trap Release

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We study the nonequilibrium dynamics of a Tonks-Girardeau gas released from a parabolic trap to a circle. We present the exact analytic solution of the many body dynamics and prove that, for large times and in a properly defined thermodynamic limit, the reduced density matrix of any finite subsystem converges to a generalized Gibbs ensemble. The equilibration mechanism is expected to be the same for all one-dimensional systems.

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The nonequilibrium dynamics of isolated many body quantum systems is currently in a golden age mainly due to the experiments on trapped ultracold atomic gases [1–8] in which it is possible to measure the unitary nonequilibrium evolution without any significant coupling to the environment. A key question is whether the system relaxes to a stationary state, and if it does, how to characterize from first principles its physical properties at late times. It is commonly believed that, depending on the integrability of the Hamiltonian governing the time evolution, the behavior of local observables can be described either by an effective thermal distribution or by a generalized Gibbs ensemble (GGE), for nonintegrable and integrable systems, respectively (see, e.g., [9] for a review). While this scenario is corroborated by many investigations [10–29], a few studies [30–35] suggest that the behavior could be more complicated and, in particular, can depend on the initial state.

In a global quantum quench, the initial condition is the ground state of a translationally invariant Hamiltonian which differs from the one governing the evolution by an experimentally tunable parameter such as a magnetic field. A different initial condition can be experimentally achieved [7,8] by considering the nonequilibrium dynamics of a gas released from a parabolic trapping potential. It has been shown experimentally that the spreading of correlations is ballistic for an integrable system and diffusive for a nonintegrable one [8]. However, when the gas expands in full space, for infinite time the gas clearly reaches zero density (see, e.g., [35–40] for a theoretical analysis) and it is rather confusing to distinguish thermal and GGE states. To circumvent this, Caux and Konik [41] have recently developed a new approach based on integrability to study the release of the Lieb-Liniger Bose gas [42] from a parabolic trap not in free space but on a closed circle (as sketched in Fig. 1), so that the gas has finite density. It has been numerically shown that the time averaged correlation functions are described by a GGE, apart from finite size effects [41]. A preliminary analysis for nonintegrable models has also been presented [43]. However, while this approach effectively permits one to calculate time-averaged quantities for relatively large systems (the maximum number of particles is $N = 56$ [41]), the study of the time evolution is possible but much harder and it is difficult to establish whether (and in which sense) an infinite time limit exists.

In order to overcome these limitations, we present here a full analytic solution of this nonequilibrium dynamics in the limit of strong coupling, i.e., in the celebrated Tonks-Girardeau regime [44]. We will show that, in a properly defined thermodynamic (TD) limit, the reduced density matrix of any *finite* subsystem converges for long times to the GGE one. This implies that any measurable *local* observable will converge to the GGE predictions.

Model and quench protocol.—We consider a one-dimensional Bose gas with delta pairwise interaction and in an external parabolic potential with Hamiltonian

$$H = -\frac{1}{2}\sum_{j=1}^{N}\frac{\partial^2}{\partial x_j^2} + \sum_{j=1}^{N}\frac{1}{2}\omega^2 x_j^2 + c\sum_{i\neq j}\delta(x_i - x_j), \quad (1)$$

where $c > 0$ is the coupling constant (we set $\hbar = m = 1$). The translationally invariant Lieb-Liniger model is obtained for $\omega = 0$ and on a circle of length L with periodic boundary conditions (PBC). While Ref. [41] covers numerically arbitrary c, to make an analytic progress

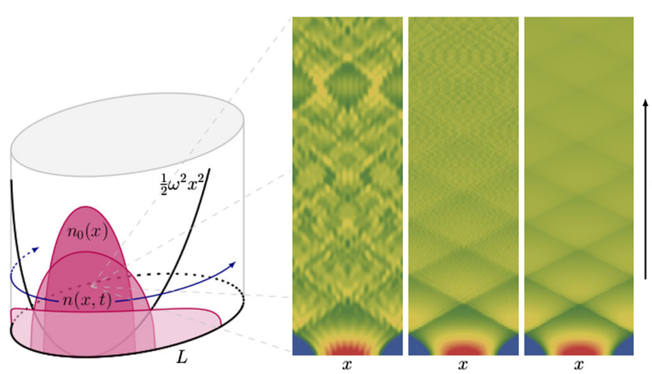

FIG. 1 (color online). Left: Sketch of the trap release dynamic in a circle. Right: Color plot of the numerical calculated density evolution for $N = 10, 100, \infty$ (from left to right) at $N/L = 1/2$ and $\omega N = 5$.

we consider the strong-coupling limit of impenetrable bosons $c \to \infty$, corresponding also to the low density $n \equiv N/L \ll 1$ regime for any c [42].

For a trap release, the initial state is a Tonks-Girardeau gas confined by a parabolic potential, i.e., the ground state of Eq. (1) for a fixed ω. Following [44], the many body wave function for the ground state of N impenetrable bosons is

$$\Psi_B(x_1, \ldots, x_N) = \prod_{i<j} \mathrm{sgn}(x_j - x_i)\Psi_F(x_1, \ldots, x_N), \quad (2)$$

where $\Psi_F(x_1, \ldots, x_N)$ is the ground-state function of N free fermions in the parabolic potential, i.e., the Slater determinant $\det_{i,j}\chi_j(x_i)$ with the eigenstates of the harmonic oscillator

$$\chi_j(x) = \frac{1}{\sqrt{2^j j!}}\left(\frac{\omega}{\pi}\right)^{1/4} e^{-\omega x^2/2} H_j(\sqrt{\omega}x), \quad (3)$$

and $H_j(z)$ the Hermite polynomials. In this fermionic language, the time evolution governed by the Hamitonian (1) with $\omega = 0$ is obtained by expanding the one-particle states in the free-wave basis, i.e. ($k = 2\pi m/L$)

$$\chi_j(x) = \sum_k A_{k,j}\frac{e^{-ikx}}{\sqrt{L}}, \qquad A_{k,j} = \int_{-L/2}^{L/2} dx \chi_j(x)\frac{e^{ikx}}{\sqrt{L}}. \quad (4)$$

We now make the only crucial *physical* assumption: we impose that the space initially occupied by the trapped gas as a whole is within the external box of length L; i.e., before the quench the PBC are irrelevant for the gas which only "sees" the parabolic trap. This condition is what allows us to talk about *release* of the gas and requires the number of particles N to be smaller than the first level of the parabolic potential that is affected by PBC. In the TD limit, for large quantum numbers, $|\chi_N(x)|^2$ is the semiclassical probability density at the corresponding energy that tends to zero for $|x| > \ell/2$ with ℓ the classical cloud dimension $\ell = 2\sqrt{2N/\omega}$. In simpler words, this means that the classical extension of the gas in the trap ℓ must be smaller than the box size L.

To have a well-defined TD limit, we should consider N, $L \to \infty$ at fixed density $n \equiv N/L$ and, at the same time, $\omega \to 0$ with ωN constant (fixed initial density), as in [41]. In terms of these quantities the gas release condition $\ell < L$ reads $\sqrt{N\omega} > 2\sqrt{2}n$ and the coefficients $A_{k,j}$ can be calculated extending the integration in Eq. (4) to $\pm\infty$, obtaining

$$A_{k,j} = i^j\sqrt{\frac{2\pi}{\omega L}}\chi_j(k/\omega). \quad (5)$$

Also, the infinite time limit should be handled with care. Indeed, in this quench, a stationary behavior is possible because of the interference of the particles going around the circle L many times (see Fig. 1); i.e., to observe a stationary value we must require $vt \gg L$ (the speed of sound is $v = \sqrt{2\omega N}$ in our normalization). This is very different from equilibration in standard global quenches where the time should be such that the boundaries are not reached (see, e.g., [17]) in order to avoid revival effects. In this problem the revival scale is $t_r \propto L^2$ and so the infinite time limit in which a stationary behavior can be achieved is $t/L \to \infty$ provided $t/L^2 \to 0$. The importance of the TD and long time limits to get a stationary behavior is already evident from the time evolution of the density profile in Fig. 1.

One-particle problem.—In fermion language, the time-dependent many body state is the Slater determinant of the time evolved one-particle initial eigenfunctions [i.e., the solution of the Schrödinger equation $i\partial_t\Phi_j(x,t) = H_F\Phi_j(x,t)$ with $\Phi_j(x,0) = \chi_j(x)$ and H_F the single-particle free Hamiltonian with PBC]. These time evolved wave functions can be calculated from Eqs. (4) and (5) obtaining

$$\Phi_j(x,t) = \sum_{p=-\infty}^{+\infty} \Phi_j^\infty(x + pL, t), \quad (6)$$

where

$$\Phi_j^\infty(x,t) = \frac{(1 - i\omega t)^{j/2} e^{-i[t\omega^2 x^2/2(1+\omega^2 t^2)]}}{(1 + i\omega t)^{(j+1)/2}}\chi_j\left(\frac{x}{\sqrt{1 + \omega^2 t^2}}\right) \quad (7)$$

is the time evolved eigenfunction in infinite space which agrees with the result in [36]. The boson-fermion mapping remains valid for the time-dependent problem [45].

Time evolution of the density profile.—We start the analysis of the many body problem from the density profile $n(x,t) = \sum_j |\Phi_j(x,t)|^2$ which shows clearly how a nonzero stationary value can be achieved in a trap release experiment. From Eq. (7) we have for arbitrary time, N, L, ω,

$$n(x,t) = \frac{1}{\sqrt{1 + \omega^2 t^2}} \sum_{p,q=-\infty}^{\infty} e^{i[\omega^2 t/2(1+\omega^2 t^2)][(x+pL)^2 - (x+qL)^2]} \times \sum_{j=0}^{N-1} \chi_j\left(\frac{x + pL}{\sqrt{1 + \omega^2 t^2}}\right)\chi_j\left(\frac{x + qL}{\sqrt{1 + \omega^2 t^2}}\right), \quad (8)$$

which, in the TD limit, because of the strongly oscillating phase factor, reduces to the diagonal part $p = q$,

$$n(x,t) = \frac{1}{\sqrt{1 + \omega^2 t^2}} \sum_{p=-\infty}^{\infty} \sum_{j=0}^{N-1} \left|\chi_j\left(\frac{x + pL}{\sqrt{1 + \omega^2 t^2}}\right)\right|^2, \quad (9)$$

and can be rewritten in terms of the TD limit of the particle density at initial time $n_0(x) = (\sqrt{2N\omega - \omega^2 x^2})/\pi$ as

$$n(x,t) = \frac{1}{\sqrt{1 + \omega^2 t^2}} \sum_{p=-\infty}^{\infty} n_0\left(\frac{x + pL}{\sqrt{1 + \omega^2 t^2}}\right), \quad (10)$$

In Figs. 1 and 2 we show the numerically calculated time-dependent density for finite but large N which perfectly agrees with the above TD prediction for any time.

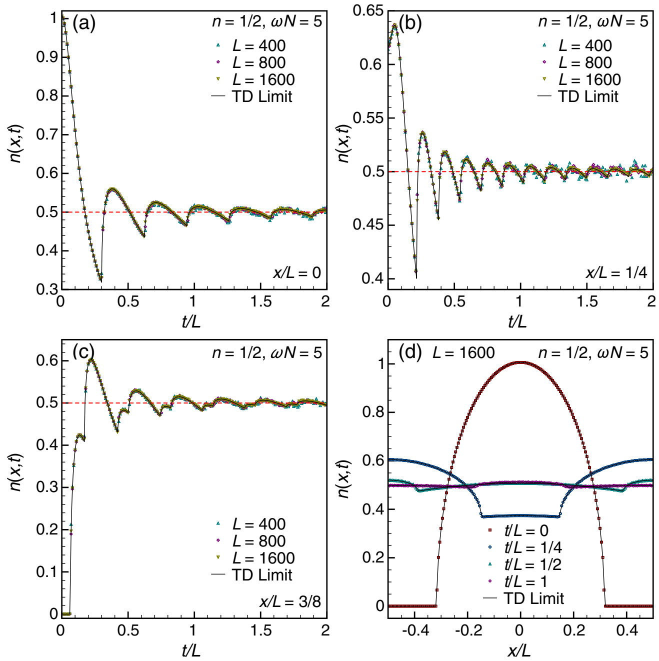

FIG. 2 (color online). (a)–(c) Time evolution of the density $n(x, t)$ for different x/L and sizes. Dashed red lines indicate the equilibration value N/L at infinite time. (d) Density profile for $L = 1600$ at different rescaled times t/L. Symbols are the exact dynamics for finite N, while full black lines are the TD limit.

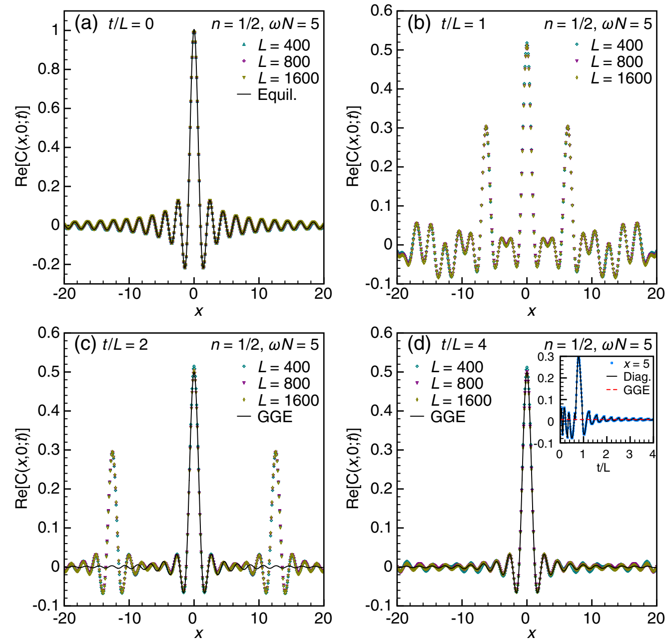

FIG. 3 (color online). (a)–(d) Snapshots of the correlation $\mathrm{Re}[C(x, 0; t)]$ at different rescaled times t/L and sizes. For $t/L = 0$ the full line is the initial correlation in the TD limit, i.e., $C(x, 0) = \sin[\sqrt{2\omega N}x]/\pi x$ valid for $x \ll L$. The full line for $t/L = 2$, 4 is the stationary value in Eq. (12). As time increases, two symmetric peaks are *expelled* from the central region. The inset in (d) shows the evolution for fixed $x = 5$ and $L = 1600$: after the moving peak has been expelled, the correlation is damped in time and converges to the GGE.

The two-point fermionic correlator $C(x, y; t) \equiv \langle \Psi^\dagger(x, t)\Psi(y, t)\rangle$ is given by

$$C(x, y; t) = \sum_{j=0}^{N-1} \Phi_j^*(x, t)\Phi_j(y, t). \qquad (11)$$

The numerical determination of this correlation function for finite N is reported in Fig. 3, showing the approach to the infinite time limit [46]

$$C(x, y; t \to \infty) = 2n \frac{J_1\left[\sqrt{2\omega N}(x - y)\right]}{\sqrt{2\omega N}(x - y)}, \qquad (12)$$

with $J_1(z)$ the Bessel function.

Reduced density matrix and the GGE.—For a closed system evolving under Hamiltonian dynamics, the existence of a stationary state may seem paradoxical because the whole system is always in a pure state and cannot be described by a mixed state at infinite time. This "paradox" is solved in the reduced density matrix formalism: given a space interval A, the reduced density matrix is $\rho_A(t) = \mathrm{Tr}_B\rho(t)$, where B is the complement of A and $\rho(t) = |\Psi(t)\rangle\langle\Psi(t)|$ is the density matrix of the whole system. With some abuse of language, we say that a system becomes stationary if, after the TD limit is taken for the whole system, the limit $\rho_{A,\infty} = \lim_{t\to\infty}\rho_A(t)$ exists for any finite A [17]. Furthermore, we say that a system is described by a statistical ensemble with density matrix ρ_E if the reduced density matrix $\rho_{A,E} \equiv \mathrm{Tr}_B\rho_E$ equals $\rho_{A,\infty}$.

For a gas of free fermions, by means of the Wick theorem, any observable can be obtained from the two-point correlator. The construction of ρ_A in terms of $C(x, y)$ in continuous space has been detailed in [47] (generalizing the lattice approach [48]). As a crucial point, the nonlocal transformation mapping the Tonks-Girardeau gas to free fermions is local within any given *compact* subspace; i.e., the bosonic degrees of freedom within A can be written only in terms of fermions in A. This is analogous to lattice models such as the Ising chain [16–18]. Thus, if for finite x, y, $C(x, y; t \to \infty)$ is described by a statistical ensemble, also ρ_A will be and consequently the expectation value of any observable local within A.

Because of integrability, it is natural to expect that Eq. (12) should be described by a GGE:

$$\rho_{\mathrm{GGE}} = Z^{-1}e^{-\sum \lambda_i I_i}, \qquad (13)$$

with $\{I_i\}$ a complete set of local integrals of motion and λ_i Lagrange multipliers fixed by the conditions $\langle\Psi_0|I_i|\Psi_0\rangle = \mathrm{Tr}[\rho_{\mathrm{GGE}} I_i]$, with $|\Psi_0\rangle$ the many body initial state. However, for free fermions, one can work with the momentum occupation modes $\hat{n}_k = c_k^\dagger c_k$ which are nonlocal

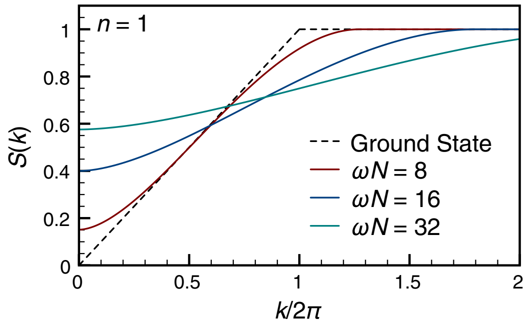

FIG. 4 (color online). The GGE structure factor $S(k)$ as a function of $k/2k_F$ ($k_F = \pi n$) for different initial trap potentials ωN compared with the ground-state one (dashed line).

integrals of motion, but can be written as linear combinations of local integrals of motion [28]. In the TD limit, the initial values of $\hat{n}_k$ are

$$\langle \Psi_0 | \hat{n}_k | \Psi_0 \rangle = \sum_{j=0}^{N-1} |A_{k,j}|^2 \simeq \frac{2}{L}\sqrt{\frac{2N}{\omega}}\sqrt{1-\frac{k^2}{2\omega N}}, \qquad (14)$$

and zero if the argument of the square root is negative. In the GGE we have $\mathrm{Tr}[\rho_{\mathrm{GGE}}\hat{n}_k] = (e^{\lambda_k}+1)^{-1}$, and equating the two, the λ_k are derived. It is now straightforward to show that $C(x, y)$ in the GGE equals the infinite time limit of trap release in Eq. (12) [46]. This shows that all stationary quantities of the released gas are described by a GGE. Furthermore, in Ref. [19] it has been shown that all nonequal time stationary properties are always determined by the same ensemble describing the static quantities, and so, even in our case, they are encoded solely in the GGE.

Structure factor in the GGE.—The structure factor $S(k)$ is the Fourier transform of the density-density correlation $\langle \hat{n}(x,t)\hat{n}(0,t)\rangle$. In any ensemble which is diagonal in the Fourier modes, in the TD limit the structure factor can be written in terms of occupation modes n_k as

$$1 - S(k) = \frac{L}{N}\int \frac{dq}{2\pi} n_q n_{k-q} = \frac{4\sqrt{2}n}{\pi\sqrt{\omega N}} f\left(\frac{k}{\sqrt{2\omega N}}\right), \qquad (15)$$

where the right-hand side is obtained using the GGE n_k given in Eq. (14). Here $f(x) = [(4+x^2)E(1-4/x^2) - 8K(1-4/x^2)]|x|/6$ if $|x| < 2$ and zero otherwise, where $E(z)$ and $K(z)$ are standard elliptic functions and $f(0) = 4/3$. $S(k)$ turns out to be an even function of k and monotonic for $k > 0$. The plot of $S(k)$ for different initial trapping potentials is reported in Fig. 4. $S(k)$ resembles the one found numerically in [41] for the Lieb-Liniger gas. Because of the trap release constraint $\sqrt{N\omega} > 2\sqrt{2}n$, we have $S(k) > S(0) \geq 1 - 8/3\pi = 0.151174\ldots$. This calculation shows how easy it is to obtain GGE predictions without solving the full nonequilibrium dynamics.

The bosonic two-point function or one-body density matrix $C_B(x, y; t) \equiv \langle \hat{\Phi}^\dagger(x,t)\hat{\Phi}(y,t)\rangle$ [with $\hat{\Phi}(y,t)$ bosonic annihilation operator] is a nontrivial quantity whose calculation presents difficulties also in thermal equilibrium [49]. However, using the approach in [50], the computation is easy for large time and in the TD limit obtaining [46]

$$C_B(x, y; t \to \infty) = C(x, y; t\to\infty)e^{-2n|x-y|}, \qquad (16)$$

with $C(x, y; t\to\infty)$ the fermion correlator in Eq. (12). For small distances, $C_B(x, y; t\to\infty)$ shows a singular behavior of the form $|x-y|$, which is different from its thermal counterpart $|x-y|^3$ [49]. This behavior is strictly valid only in the TD limit because, for any finite N, at very small distances $C_B(x, y; t\to\infty)$ crosses over to $|x-y|^3$ as expected from general arguments [49]. This finite N crossover is numerically demonstrated in [46]. Consequently, the momentum distribution function has a large momentum tail of the form k^{-2} which crosses over to the standard k^{-4} for even larger k. This large-momentum crossover should be a measurable signature of the GGE.

Trap to trap release.—The case of a Tonks-Girardeau gas released not in a periodic system but in a larger harmonic trap has been solved by Minguzzi and Gangardt [36] who showed that the system oscillates forever without relaxation. However, even in this case, it is simple to see that the time-averaged two-point correlations (and hence by Wick theorem any observable) are still described by a GGE.

Conclusions.—In this Letter we solved analytically the nonequilibrium dynamics of a Tonks-Girardeau gas following a trap release to a periodic geometry as in Fig. 1. We prove that for long time and in the TD limit, any finite subsystem becomes stationary and its behavior is described by a GGE. This provides the first analytic proof of a GGE for an inhomogeneous initial state. We stress that the mechanism responsible for the equilibration is very different from the one in a global quantum quench since in the trap release it is due to the interference of the particles going around the circle many times. This equilibration mechanism is expected to be the same for any one-dimensional gas released into a circle.

Apart from the *per se* experimental interest [7,8], these results represent a first step towards a complete analytical understanding of the famous quantum Newton cradle [2] at least in the Tonks-Girardeau limit.

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