Interaction quenches in the Lieb–Liniger model

Márton Kormos, Aditya Shashi, Yang-Zhi Chou, and Adilet Imambekov
Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA
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We obtain exact results on interaction quenches in the 1D Bose gas described by the integrable Lieb-Liniger model. We show that in the long time limit integrability leads to significant deviations from the predictions of the grand canonical ensemble and a description within the generalized Gibbs ensemble (GGE) is needed. For a non-interacting initial state and arbitrary final interactions, we find that the presence of infinitely many conserved charges generates a non-analytic behavior in the equilibrated density of quasimomenta. This manifests itself in a dynamically generated Friedel-like oscillation of the non-local correlation functions with interaction dependent oscillation momenta. We also exactly evaluate local correlations and the generalized chemical potentials within GGE.

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Whether and how an isolated quantum system equilibrates or thermalizes are fundamental questions in understanding non-equilibrium dynamics. The answers can also shed light on the applicability of quantum statistical mechanics to closed systems. While these questions are very hard to study experimentally in the condensed matter setup, they have become accessible in ultracold quantum gases due to the recent experimental advances [1]. Thanks to their unprecedented tunability, ultracold atomic systems allow for the study of non-equilibrium quantum dynamics of almost perfectly isolated strongly correlated many-body systems in a controlled way. These experiments [2, 3] triggered a revival of theoretical studies on issues of thermalization [4]. Fundamental questions include whether stationary values of local correlation functions are reached in a system brought out of equilibrium, and if so, how they can be characterized. Can conventional statistical ensembles describe the state? Is there any kind of universality in the steady state and the way it is approached?

The absence of thermalization of a 1D bosonic gas reported in [3] brought to light the special role of integrability. The lack of thermalization was attributed to the fact that the system was very close to an integrable one, the Lieb–Liniger (LL) model [5], which is the subject of our Letter. The dynamics of integrable systems is highly constrained by the presence of a large number of so-called conserved charges in addition to the total particle number, momentum, and energy. Thus integrable systems are not expected to thermalize. Following the ideas of the subjective statistical mechanics of Jaynes [6], the so-called generalized Gibbs ensemble (GGE) was proposed [7] to capture the long-time behavior of integrable systems brought out of equilibrium. This ensemble is the least biased statistical representation of the system once the conserved charges \( \{Q_m\} \) are taken into account. The density matrix is

\[
\hat{\rho}_{\text{GGE}} = \frac{e^{-\sum_m \beta_m Q_m}}{Z_{\text{GGE}}},
\]

where the generalized “chemical” potentials \( \{\beta_m\} \) are fixed by the expectation values \( \langle Q_m \rangle \), and \( Z_{\text{GGE}} = \text{Tr} \left[ e^{-\sum_m \beta_m Q_m} \right] \).

The GGE was tested and its drawbacks were analyzed by various numerical and analytical approaches [8]. However, with a few exceptions [9, 10], only models that can be mapped to quadratic bosonic or fermionic systems have been considered, where the conserved charges are given by the mode occupation numbers. While some of these models are paradigmatic, like the Ising or Luttinger models, a prominent class of non-trivial integrable systems has not been sufficiently explored, namely those solvable by the Bethe Ansatz. In these models, the conserved charges are local and cannot be expressed as mode occupations.

In this Letter, we derive experimentally testable predictions for the long time behavior of the system after an interaction quench [11, 12] in the LL model by combining its Bethe Ansatz solution and GGE. For a non-interacting initial state and arbitrary final interactions, the infinitely many conserved charges result in Friedel-like oscillations in the two-point functions, in striking contrast to the grand canonical ensemble (GCE).

The model.--- The LL model describes a system of identical bosons in 1D interacting via a Dirac-delta potential. The Hamiltonian in second quantized formulation is given by [5]

\[
\hat{H} = \int_0^L dx \left( \partial_x \hat{\psi}^\dagger \partial_x \hat{\psi} + c \, \hat{\psi}^\dagger \hat{\psi}^\dagger \hat{\psi} \hat{\psi} \right),
\]

where \( c > 0 \) in the repulsive regime we wish to study, and for brevity we have set \( \hbar = 1 \) and the boson mass to be equal to 1/2. The dimensionless coupling constant is given by \( \gamma = c/n \), where \( n = N/L \) is the density of the gas. In cold atom experiments \( \gamma \) is a function of the 3D scattering length and the 1D confinement [3, 13]. The exact spectrum and thermodynamics of the model can be obtained via Bethe Ansatz [5, 14]. Each eigenstate of the system with \( N \) particles on a ring of circumference \( L \) is characterized by a distinct set of quantum numbers \( \{I_j\} \).
that are integers (half-integers) for \( N \) odd (even). The wave function can be expressed in terms of \( N \) quasimomenta \( \{\lambda_j\} \) that satisfy a set of algebraic equations

\[
L\lambda_j + \sum_{k=1}^{N} \theta(\lambda_j - \lambda_k) = 2\pi I_j,
\]

where \( \theta(\lambda) = 2\arctan(\lambda/c) \). The expectation values of the local conserved charges can be computed as

\[
Q_m \equiv \langle \hat{Q}_m \rangle = \sum_j \lambda_j^m,
\]

in particular, the energy of a given state is simply \( E = Q_2 = \sum_j \lambda_j^2 \). The wave function is identically zero if any two of the \( \{I_j\} \) coincide, which is reminiscent of the Pauli principle for fermions. In the thermodynamic limit, a mixed state corresponding to thermal equilibrium is captured by a filling fraction \( f_1 < f < 1 \) in the space of quantum numbers. It has been shown in Ref. [10] that GGE also implies that such a description is possible. For calculations, it is more convenient to define a function \( f(\lambda) \) in terms of the quasimomenta. Unlike the case of free fermions, where the relation between \( f_1 \) and \( f(\lambda) \) is trivial, here all quasimomenta are coupled to each other by Eq. (3). Thus the density of occupied quasimomenta \( \rho^{(p)}(\lambda) \) is not independent of \( f(\lambda) \) but satisfies the integral equation \([5]\)

\[
\rho(\lambda) = \frac{1}{2\pi} \frac{d\lambda}{2\pi} \varphi(\lambda - \lambda') \rho^{(p)}(\lambda'),
\]

where the kernel \( \varphi(\lambda) = 2c/(\lambda^2 + c^2) \). Here \( \rho(\lambda) \) is the maximal allowed density of quasimomenta and \( \rho^{(p)}(\lambda) \) is normalized as \( \int d\lambda \rho^{(p)}(\lambda) = n \).

Conserved charges and the problem of moments. — The simplest way to bring a system out of equilibrium is a sudden change of one of its parameters, a quantum quench. In a cold atom setting such a quench could be achieved by a rapid change of the transverse confinement or the scattering length. We will compute the predictions of the GGE for a sudden quench of the interaction parameter, and compare them to those of the GCE. In order to describe the final state in terms of \( \rho^{(p)}(\lambda) \), one needs to find the expectation values of the conserved charges \( Q_m \) right after the quench. For \( c > 0 \), all solutions of Eq. (3) are real [14], thus finding the density \( \rho^{(p)}(\lambda) \) which reproduces these charges is equivalent to solving the problem of moments defined by

\[
Q_m = L \int d\lambda \rho^{(p)}(\lambda) \lambda^m.
\]

The first few conserved charge operators \( \hat{Q}_m \) can be written in terms of the field operator \( \hat{\psi}(x) \) as \( \hat{Q}_0 = \int dx \hat{\psi}^\dagger \hat{\psi} \), \( \hat{Q}_1 = -i \int dx \hat{\psi}^\dagger \partial_x \hat{\psi} \), and \( \hat{Q}_2 = \hat{H} \) is the Hamiltonian given by Eq. (2). Except for \( \hat{Q}_0 \) and \( \hat{Q}_1 \), the charges depend on \( c \) and their expectation values change during the quench according to their \( c \)-dependence [11]. Unfortunately, the corresponding expressions are not known explicitly for the operators \( \hat{Q}_m \) for \( m \geq 4 \) [16].

In the thermodynamic limit, the even conserved charges are expected to have the form

\[
\hat{Q}_{2m} = \int dx \left[ \text{deriv.} + A_m \gamma^m : (\hat{\psi}^\dagger \hat{\psi})^m+1 : \right],
\]

where \{deriv.\} denotes unknown terms which involve products of spatial derivatives of \( \psi(x) \) and \( \psi^\dagger(x) \) and \( : : \) denotes normal ordering. The constants \( A_m \) can be calculated comparing Eq. (7) to the semiclassical limit (\( \gamma \ll 1 \)) where the expressions for the conserved charges are known [17]. The constants \( A_m \) satisfy a certain recursion relation, which can be solved to obtain \( A_m = 2m(2m - 1)!!/(m + 1)! \) [23]. Note that assuming an even \( \rho^{(p)}(\lambda) \), as in the ground state, we keep only the even charges.

Universal semicircle solution. — If the initial state is in a pure non-interacting BEC (although we expect our results to be also valid for small initial interactions), then the expectation values of the unknown derivative terms in Eq. (7) vanish. Thus the conserved charges are given by \( Q_{2m}/L \approx A_m \gamma^m : (\hat{\psi}^\dagger \hat{\psi})^m+1 : \approx A_m \gamma^{2m+1} \gamma^m \), where in the last step we used the fact that the local correlators \( \langle \hat{\psi}(x) \hat{\psi}(y) \rangle \rightarrow n^m \) as \( \gamma \rightarrow 0 \). We are left with the following problem of moments:

\[
\int d\lambda \rho^{(p)}(\lambda) \lambda^m = 2m(2m - 1)!! \gamma^m \sum_{m=0}^\infty \frac{\lambda^m}{(m+1)!},
\]

which has the unique solution

\[
\rho^{(p)}(\lambda) = \frac{1}{\pi \sqrt{\gamma}} \sqrt{1 - \lambda^2 / \lambda_*^2}, \quad \lambda_* = 2n \sqrt{\gamma}.
\]

on the interval \([\lambda_-, \lambda_*] \) and zero otherwise (see inset of Fig. 1). Using Eqs. (5) we can determine \( f(\lambda) \):

\[
f(\lambda) = \frac{1 - (\lambda/\lambda_*)^2}{\sqrt{(1 + 4 \gamma^2 - (\lambda/\lambda_*)^2)^2 + 4 \gamma}}.
\]

We emphasize that the existence of the sharp edge of support in Eq. (9) is a direct consequence of our accounting for an infinite number of conserved charges. Keeping any finite number within GGE would smear the sharp edge.

Correlation functions in the final state. — Knowing the filling fraction \( f(\lambda) \) allows us to calculate some of the correlation functions. First we calculate local correlators exactly using the results of Ref. [18] which give analytic expressions for the local two and three-point correlators for arbitrary states that are captured by a
continuous \( f(\lambda) \). We compute \( g_2 = \langle (\hat{\psi}^\dagger \hat{\psi})^2 \rangle / n^2 \) and \( g_3 = \langle (\hat{\psi}^\dagger \hat{\psi})^3 \rangle / n^3 \) both for both for GGE and the GCE by using the appropriate \( f(\lambda) \). In the latter only the energy and the particle densities are fixed to be the same as for the GGE, which determines the temperature and the chemical potential. The results are shown in Fig. 1. For interactions not too strong, the GGE results are very close to the values for GCE which slightly underestimates \( g_2 \) and overestimates \( g_3 \). The deviation is bigger for \( g_3 \) and grows with \( \gamma \). Both GGE and GCE results are consistent with the outcomes of recent numerical simulation [11]. We conclude that the local correlators above are too simple to effectively distinguish between the various ensembles.

Note, however, that the densities of filled states \( \rho^{(p)}(\lambda) \) are very different for the GGE and the GCE, see the inset of Fig. 1. Remarkably, the semicircle distribution exhibits a non-analytic square root singularity at the edges, which has immediate consequences for the behavior of the nonlocal correlation functions. In analogy with the Friedel oscillations, which appear due to the existence of a sharp Fermi surface, we expect that the non-analyticity of \( \rho^{(p)}(\lambda) \) at \( \lambda_0 \) will result in the oscillating behavior of nonlocal correlation functions. Unlike the period of conventional Friedel oscillations which depends only on the average density, the period of these dynamically generated Friedel oscillations also depends on the interaction strength. The characteristic momentum \( k_0 \) which plays the role of the Fermi momentum can be calculated using standard techniques [5, 14], and is plotted in the inset of Fig. 2. While we cannot explicitly calculate the nonlocal correlation functions for arbitrary final interactions, below we present detailed results for strong final interactions which support this picture.

**Strongly interacting final state.**— For large coupling the system is effectively in the fermionized regime, since the largest quasimomentum \( \lambda_0 \) scales only as \( \sim \sqrt{\gamma} \) and thus the convolution term in Eq. (3a) depending on the kernel \( \varphi(\lambda) \) can be neglected. The function \( f(\lambda) \) takes the form

\[
\begin{align*}
  f(\lambda) &\approx \frac{2}{\sqrt{\gamma}} \sqrt{1 - \left(\frac{\lambda}{\lambda_0}\right)^2}.
\end{align*}
\]

Bosonic correlation functions can be calculated by first fermionizing the field operators using Jordan–Wigner strings, \( \hat{\psi}(x) = \exp[\pi \int x^\infty \hat{\psi}_F^\dagger(z) \hat{\psi}_F(z) dz] \hat{\psi}_F(x) \), and then exploiting free fermionic correlators of \( \hat{\psi}_F \) in the large \( \gamma \) regime. Let us consider the equal time Green’s function

\[
G(x) = \frac{\langle \hat{\psi}^\dagger(x) \hat{\psi}(0) \rangle_{SC}}{\langle \hat{\psi}^\dagger(x) \hat{\psi}(0) \rangle_{SC}},
\]

where SC denotes averaging over the semi-circle distribution of Eq. (11). We proceed by introducing a lattice discretization \( a \ll 1/n, x = (m + 1)a \) and recasting the correlator as

\[
G(x) = \left\langle \hat{\psi}_F^\dagger(x) \prod_{k \leq m} \left[ 1 - 2 \hat{\psi}_F^\dagger(ka) \hat{\psi}_F(ka) \right] \hat{\psi}_F(a) \right\rangle.
\]

The long chain of operators is now amenable to a Wick expansion using as a building block the fermionic two point function given by the Fourier transform of the distribution (11), \( G_F(x) = \int \frac{d\lambda}{2\pi} f(\lambda) e^{i \lambda x} = 2n J_0(\lambda x)/(\lambda x) \), where \( J_0(x) \) is the Bessel function of the first kind. The Wick expansion of Eq. (13) can be recast as a Fredholm-like determinant since the correlator of \( 2n \) fields can be represented as a deter-
chemical potential $\beta$ results $\approx \gamma$ canonical prediction (solid, red) and analytical large exponential decay in the thermal state.

For the GGE case we use the arbitrary function $g$. The result, $\lambda$ changes from 25 to 2 as $\lambda \to \pm \lambda_\ast$, as $\varepsilon(\lambda) \sim \frac{1}{2} \log[1 - (\lambda/\lambda_\ast)^2]$. This divergence results in the large $m$ behavior of the chemical potentials as

$$\beta_{2m} \approx \frac{1}{2m\lambda_{2m}^2} = \frac{1}{2m(4n^2\gamma)^m}.$$ (15)

None of them diverges but since there are infinitely many of them, their collective behavior renders $\varepsilon(\lambda)$ divergent for $\lambda \geq \lambda_\ast$. This creates a “Fermi edge” by constraining $\rho(\lambda)$ to have a finite range of support. This mechanism is markedly different from the case of the ground state, where the divergence of a finite number of chemical potentials, as the temperature goes to zero, results in a step distribution function.

**Summary.**— We studied the large time behavior of the post interaction quench state in the Lieb-Liniger model using analytic techniques by combining the generalized Gibbs ensemble and Bethe Ansatz integrability of the model. For a non-interacting initial state and arbitrary final interactions, the infinitely many conserved charges result in Friedel-like oscillations in the two-point functions with interaction dependent momentum. This is in striking contrast to the behavior of the thermalized system and provides a smoking gun signal for cold atom experiments. We also exactly evaluated local correlations and the generalized chemical potentials within GGE.

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[23] Alternatively, one can establish the values of $A_m$ by using the limiting semicircle behavior of the ground state solution in the weakly interacting regime [5], and evaluating $Q_m$ according to Eq (6).