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Interaction quenches in the one-dimensional Bose gas

Márton Kormos,1,2,3,4,* Aditya Shashi,1,5 Yang-Zhi Chou,1 Jean-Sébastien Caux,6 and Adilet Imambekov1,1

1Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA
2Dipartimento di Fisica dell’Università di Pisa and INFN, 56127 Pisa, Italy
3Department of Theoretical Physics, Budapest University of Technology and Economics, 1111 Budapest, Budaöri út 8, Hungary
4MTA-BME “Momentum” Statistical Field Theory Research Group, 1111 Budapest, Budaöri út 8, Hungary
5Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA
6Institute for Theoretical Physics, University of Amsterdam, Science Park 904, Postbus 94485, 1090 GL Amsterdam, The Netherlands

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I. INTRODUCTION

Whether and how an isolated quantum system equilibrates or thermalizes are fundamental questions in understanding nonequilibrium 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 recent experimental advances.3 Thanks to their unprecedented tunability, ultracold atomic systems allow for the study of nonequilibrium quantum dynamics of almost perfectly isolated strongly correlated many-body systems in a controlled way. These experiments have triggered a revival of theoretical studies on issues of thermalization.11–27 The list of 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?3

The absence of thermalization of a 1D bosonic gas reported in Ref. 3 brought to light the special role of integrability. The observed lack of thermalization was attributed to the fact that the system was very close to an integrable one, the Lieb-Liniger (LL) model28 which is the subject of our paper. The dynamics of integrable systems are highly constrained by the presence of a large number of conserved charges29 in addition to the total particle number, momentum, and energy, thus they are not expected to thermalize. The so-called generalized Gibbs ensemble (GGE) was proposed 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 \( \{ \hat{Q}_m \} \) are taken into account. The density matrix is

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

where the generalized “chemical potentials” \( \{ \beta_m \} \) are fixed by the expectation values \( \langle \hat{Q}_m \rangle \) in the initial state, and \( Z_{\text{GGE}} = \text{Tr}[e^{-\sum_m \beta_m \hat{Q}_m}] \). The GGE proposal was tested successfully by various numerical and analytic approaches.20–23

Recently, locality has emerged as a crucial ingredient in the understanding of equilibration and the meaning of a steady state.24 While the whole system starting in an initial pure state clearly cannot evolve into a mixed state, its subsystems are fully described by a reduced density matrix obtained by tracing out the rest of the system that acts as a bath for the subsystem. There is substantial evidence that this density matrix is thermal for generic systems and given by the GGE for integrable systems. In Ref. 16 it has been shown for the Ising chain in a transverse field that the infinite time limit of the reduced density matrix of a spatial subsystem is equal to the reduced density matrix obtained from \( \hat{\rho}_{\text{GGE}} \), and thus the GGE completely captures all observables localized in the subsystem. Naturally, it is the local conserved charges that are to be used in the GGE density matrix.

The GGE was studied mostly in models which can be mapped to quadratic bosonic or fermionic systems 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 nontrivial integrable systems has not been sufficiently explored, namely those solvable by the Bethe ansatz (BA). In these models, the local conserved charge operators are usually known but cannot be expressed as mode occupations.

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Reference 22 focused on integrable quantum field theories with diagonal scattering and demonstrated that the long-time limit of expectation values are given by a GGE, assuming a special initial state corresponding to an integrable boundary state. In Ref. 25 it was shown for BA integrable models that in the thermodynamic limit the time evolution of local observables after a quantum quench is captured by a saddle point state, and that $t \to \infty$ asymptotic values are given by their expectation values in this state. The saddle point state can be determined using the expectation values of the charges in the initial state which connects this method with the GGE approach. Recently there has been progress on the GGE in the thermodynamic limit (TDL), which quantifies the distribution of quasimomenta. In the finite volume case periodic boundary conditions force the quasimomentum to be solutions of the Bethe ansatz equations:

$$\phi(x_j; \{\lambda\}) \sim \sum_{P \in S_N} (-1)^{|P|} e^{i P \cdot \{x_j\}} \prod_{j \neq k} (\lambda_j - \lambda_k - ic \epsilon(x_j - x_k)).$$

where $\{\lambda\}$ is the set of $N$ quasimomenta, $\epsilon(x)$ is the sign function, and the $P \in S_N$ are permutations. In the finite volume case periodic boundary conditions force the quasimomenta to be solutions of the Bethe ansatz equations:

$$e^{i \lambda_j} \prod_{k \neq j} (\lambda_j - \lambda_k - ic) = 1, \quad j = 1, \ldots, N.$$  

In the repulsive case ($c > 0$) considered here all solutions of the Bethe equations are given by real quasimomenta. The eigenvalues of the mutually commuting local conserved charges can be computed as (\hat{Q}_m) = \sum_{j} \lambda_j^m, in particular, the energy is simply $E = \langle \hat{Q}_2 \rangle = \sum_{j} \lambda_j^2$. It is useful to define the density of roots, $\rho_{LL}(\lambda_j) = 1/(L(\lambda_{j+1} - \lambda_j)),$ which quantifies the distribution of quasimomenta. In the thermodynamic limit (TDL), $N, L \to \infty$ with $n = N/L$ fixed, the function $\rho_{LL}(\lambda)$ becomes smooth and can describe even mixed states. The expectation values of the conserved charges in a state having quasimomentum distribution $\rho_{LL}(\lambda)$ are given by

$$\langle \hat{Q}_m \rangle = L \int d\lambda \, \rho_{LL}(\lambda) \lambda^m.$$  

All quasioccupancies are coupled to each other by the Bethe equations and thus $\rho_{LL}(\lambda)$ as well as the density of “holes” satisfies integral equations, the thermodynamic Bethe ansatz (TBA) equations. This approach was developed for thermal equilibrium but it can be generalized to the case of the GGE.

### III. DIVERGENCE OF THE LOCAL CONSERVED CHARGES

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 sudden quench of the interaction parameter $c$ starting from the ground state of the $c = 0$ system, a pure noninteracting BEC (although we expect our results to be also valid for small initial interactions) and compare them with those of the grand canonical ensemble (GCE).

In order to describe the final state in terms of the distribution $\rho_{LL}(\lambda)$, one needs to find the expectation values of the eigenfunctions $\phi(x_j)$ of $\hat{H}$ satisfy the boundary condition

$$\left( \frac{\partial}{\partial x_j} - \frac{\partial}{\partial x_k} - c \right) \phi(x_1, \ldots, x_N) \bigg|_{x_j = x_k + 0} = 0,$$

whenever the coordinates of two particles coincide, thus the wave functions have cusps.

The $N$-particle coordinate space eigenfunctions are superpositions of plane waves,

$$\phi(x_j; \{\lambda\}) \sim \sum_{P \in S_N} (-1)^{|P|} e^{i P \cdot \{x_j\}} \prod_{j \neq k} (\lambda_j - \lambda_k - ic \epsilon(x_j - x_k)).$$

where $\{\lambda\}$ is the set of $N$ quasimomenta, $\epsilon(x)$ is the sign function, and the $P \in S_N$ are permutations. In the finite volume case periodic boundary conditions force the quasimomentum to be solutions of the Bethe ansatz equations:

$$e^{i \lambda_j} \prod_{k \neq j} (\lambda_j - \lambda_k - ic) = 1, \quad j = 1, \ldots, N.$$  

The exact spectrum and thermodynamics of the model can be obtained via Bethe ansatz. The many-body
conserved charges $Q_m$ right after the quench, i.e., in the BEC-like ground state of free bosons. The density $ρ_{\text{LL}}(\lambda)$ is then found, in principle, by solving the problem of moments defined by Eq. (9). The first few $Q_m$ can be written in terms of the field operator as

$$
\hat{Q}_0 = \int dx \hat{\psi}^\dagger \hat{\psi},
$$

$$
\hat{Q}_1 = -i \int dx \hat{\psi}^\dagger \partial_x \hat{\psi},
$$

$$
\hat{Q}_2 = \hat{H},
$$

where $H$ is the Hamiltonian given by Eq. (3). Unfortunately, similar second quantized expressions do not exist for the operators $Q_m$ for $m \geq 4$. More importantly, their expectation values can be shown to diverge in almost all states other than the eigenstates of $\hat{H}$. The reason is that their first quantized expressions contain products of Dirac-δ and higher derivatives, and are only meaningful when evaluated on a wave function satisfying the cusp condition (5). Clearly any eigenfunction of the Hamiltonian with a different coupling $c$, including the BEC wave function, will violate this condition. Note that although its expectation value is finite, even the action of the Hamiltonian is singular on such a state as it generates Dirac-δ [see Eq. (2)]. The fact that the higher charges diverge can also be verified for $N = 2$ particles and quenches from the $c = 0$ ground state by explicitly calculating the overlaps between the eigenstates and the initial state which is a constant. The overlaps scale as $\lambda^{-2}$ for large $\lambda$ which implies that $\langle \hat{Q}_m \rangle$ diverge for $m \geq 4$.35

Based on Eq. (9) the diverging expectation values of the charges imply in general that the density $ρ_{\text{LL}}(\lambda)$ has a $\lambda^{-4}$ power-law tail instead of the usual exponential fall-off.

The fact that the post-quench expectation values of the conserved charges are divergent renders the GGE ill-defined. We expect these divergences to be a generic phenomenon for sudden interaction quenches of continuum integrable models having contact interactions. This implies that the GGE prescription needs to be modified for a large and important class of the continuum integrable systems, which deserves further study.

IV. $q$-BOSON REGULARIZATION

A. The $q$-boson hopping model

To circumvent the problem of divergences we regularize them by considering an integrable lattice regularization of the LL model, the so-called $q$-boson hopping model36 (see also Ref. 37). The discussion below follows some parts of Ref. 38.

The Hamiltonian of the $q$-boson hopping model is

$$
H_q = -\frac{1}{\delta^2} \sum_{j=1}^{M} (B_j^\dagger B_{j+1} + B_{j+1}^\dagger B_{j} - 2N_j),
$$

where $\delta$ is the lattice spacing of the lattice of length $M$ having periodic boundary conditions. The operators $B_j, B_j^\dagger$ and the number operator $N_j = N_j^\dagger$ satisfy the $q$-boson algebra

$$
B_j B_{j+1}^\dagger = q^{-2} B_{j+1}^\dagger B_{j} = 1,
$$

$$
[N_j, B_j] = -B_j, \quad [N_j, B_j^\dagger] = B_j^\dagger,
$$

and operators at different sites commute.

We work with the representation on the Fock space generated by the canonically commuting lattice boson operators $b_j, b_j^\dagger$. At site $j$,

$$
b_j |m\rangle = m^{1/2} |m-1\rangle_j,
$$

$$
b_j^\dagger |m\rangle = (m+1)^{1/2} |m+1\rangle_j.
$$

The basis states of the whole lattice are given by the tensor product of the local Fock states:

$$
|0\rangle = \bigotimes_{j=1}^{M} |0\rangle_j, \quad |m\rangle = \bigotimes_{j=1}^{M} |m\rangle_j.
$$

In the local on-site Fock space the action of the local operator $N_j$ entering Eqs. (15) is identical with that of the operator $b_j^\dagger b_j$, for which

$$
N_j |m\rangle_j = m |m\rangle_j.
$$

The operators $B_{j}^\dagger$ and $B_j$ in Eqs. (15) act in the local Fock space as

$$
B_j |m\rangle_j = |m^{1/2} |m-1\rangle_j,
$$

$$
B_{j}^\dagger |m\rangle_j = |m+1^{1/2} |m+1\rangle_j,
$$

where

$$
x_q \equiv \frac{1 - q^{-2x}}{1 - q^{-2}}.
$$

Clearly $[x_q]_q \to x$ as $q \to 1$, so in the limit $q \to 1, B_j^\dagger \to b_j^\dagger$, and $B_j \to b_j$. In the Fock space representation it is possible to express the local $q$ operators as

$$
B_j = \sqrt{N_j + 1} b_j, \quad B_{j}^\dagger = b_{j}^\dagger \sqrt{N_j + 1},
$$

and give an alternative form of the commutation relation:

$$
[B_j, B_{j}^\dagger] = q^{-2N_j}.
$$

The Hamiltonian is nonpolynomial either in the $b$ or the $B$ operators, thus the model is interacting and the interaction is encoded in the deformation parameter $q$. Indeed, in the naive limit $q \to 1$ we recover the system of free bosons hopping on a lattice:

$$
H_q \to -\frac{1}{\delta^2} \sum_{j=1}^{M} (b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_{j} - 2N_j).
$$

We are interested instead in the following continuum limit: let $\delta \to 0, M \to \infty$, and $q \to 1$, while $L$ and $c$ are kept constant:

$$
L = M\delta, \quad c/2 = \kappa \delta^{-1}, \quad \text{as} \ M \to \infty \text{and} \ \delta, \kappa \to 0,
$$

where $\kappa$ is related to $q$ as

$$
q = e^{\kappa}. \quad
$$

Defining the continuum boson fields $\hat{\psi}(x = j\delta) = \delta^{-1/2} b_j$, and using the small $\kappa$ expansion

$$
\sqrt{\frac{N_j + 1}{N_j + 1}} = 1 - \frac{\kappa}{2} N_j + \frac{\kappa^2}{24} N_j(5N_j + 4) + \cdots,
$$

we find

$$
\hat{\psi}(x) = \frac{1}{\delta} \int dx \hat{\psi}(x).
$$

and using the small $\kappa$ expansion

$$
\hat{\psi}(x) = \frac{1}{\delta} \int dx \hat{\psi}(x).
$$

(29)

$$
\hat{\psi}(x) = \frac{1}{\delta} \int dx \hat{\psi}(x).
$$

and using the small $\kappa$ expansion

$$
\hat{\psi}(x) = \frac{1}{\delta} \int dx \hat{\psi}(x).
$$
it can be shown that the $q$-boson Hamiltonian (13) becomes the LL Hamiltonian in the limit (26).

For a regularized version of the GGE we need to know the local conserved quantities of the $q$-boson model. We turn to these conserved quantities in the next subsection.

B. Local conserved charges in the $q$-boson hopping model

Integrals of motion of the $q$-boson hopping model can be constructed using the quantum inverse scattering method.\textsuperscript{31} The $L$ operator for the model is given by

$$L_j(\xi) = \left( \begin{array}{ccc} \zeta & \chi B_j^\dagger \\ \chi B_j & \zeta^{-1} \end{array} \right),$$

where $\chi = \sqrt{1 - q^{-2}} = \sqrt{1 - e^{-2\xi}}$. The monodromy matrix $T(\xi)$ is given by the matrix product of the $L$ operators over the lattice sites,

$$T(\xi) = L_M(\xi)L_{M-1}(\xi)\cdots L_1(\xi),$$

and the transfer matrix $\tau(\xi)$ is given by the trace over the matrix space of the monodromy matrix,

$$\tau(\xi) = \text{Tr} T(\xi).$$

For any $\lambda$ and $\mu$ the transfer matrices commute: $[\tau(\lambda), \tau(\mu)] = 0$, which implies that $\tau(\xi)$ is a generating function of the conserved charges. Many different sets can be generated since any analytic function of $\tau(\xi)$ can play the role of the generating function. We consider the set consisting of local charges that can be written in the form

$$I_m = \delta \sum_{j=1}^M \mathcal{J}_j^{(m)},$$

where the operators $\mathcal{J}_j^{(m)}$ act nontrivially in $m + 1$ neighboring lattice sites only. This set is obtained by the formula

$$I_m = \frac{1}{(2m)!} \frac{d^{2m}}{d \xi^{2m}} \ln[\chi^m \tau(\xi)] \bigg|_{\xi = 0}, \quad m = 1, 2, 3, \ldots$$

To give an example we quote the first two local operator densities $\mathcal{J}_j^{(1)}$ and $\mathcal{J}_j^{(2)}$:

$$\mathcal{J}_j^{(1)} = \frac{1}{\delta} \chi^2 B_j B_{j+1},$$

$$\mathcal{J}_j^{(2)} = \frac{1}{\delta} \chi^2 \left( 1 - \frac{\chi^2}{2} \right) \left( B_j^\dagger B_{j+2} - \frac{\chi^2}{2} B_j^\dagger B_j B_{j+1} B_{j+1} - \chi^2 B_j^\dagger B_{j+1} B_{j+1} B_{j+2} \right).$$

The charges $I_m$ are not Hermitian operators. However, using the relation $[\tau(\xi)]^\dagger = \tau(\xi^{-1})$ it can be proved that $[I_m, I_n] = 0$ for any $m, n$. For convenience, we introduce the notation

$$I_{-m} \equiv I_{m}, \quad m = 1, 2, 3, \ldots$$

As the number operator $N = \sum_j N_j = \sum_j b_j^\dagger b_j$ is non-polynomial in the $B_j^{(i)}$ operators while the charges $I_m$ are, it cannot be expressed as a finite linear combination of the $I_m$. However, $N$ commutes with any monomial containing an equal number of the creation and annihilation operators thus $[N, I_m] = 0$. It is convenient to use the notation $N \equiv I_0$. The Hamiltonian (13) can then be expressed as

$$H_q = -\frac{1}{\chi^2} \left( I_1 + I_{-1} - 2\chi^2 I_0 \right).$$

We would like to point out that the charges are not in simple one-to-one correspondence with the LL operators $\hat{Q}_m$.\textsuperscript{3}

Similarly to the LL model, the common eigenstates of all $I_m$ are defined in the $N$-particle sector by $N$ quasimomenta $\{p_j\}$ which are solutions of the $q$-boson Bethe equations:

$$e^{iM p_j} = \prod_{k=1}^N \frac{\sin \left( \frac{\pi}{2} (p_j - p_k) + i \kappa \right)}{\sin \left( \frac{\pi}{2} (p_j - p_k) - i \kappa \right)}, \quad j = 1, \ldots, N.$$ 

It is easy to see that under the limit (26) we need to rescale the quasimomenta as $\lambda_j = p_j/\delta$ in order to regain the Bethe equations of the LL model in terms of the LL rapidities $\lambda_j$. The eigenvalues of the charges are given by\textsuperscript{3}

$$I_m |\psi_N\rangle = (1 - q^{-2|m|}) \frac{1}{|m|} \sum_{j=1}^N e^{-i M p_j} |\psi_N\rangle$$

for $m = \pm 1, \pm 2, \ldots$.

We will be interested in the thermodynamic limit of the $q$-boson system, $N, M \to \infty$, with $v \equiv N/M$ fixed. In a way completely analogous to the LL case, one can introduce the quasimomentum distribution function $\rho_q(p_j)$:

$$\rho_q(p_j) = \frac{1}{M(p_{j+1} - p_j)},$$

with the normalization

$$\int_{-\pi}^{\pi} dp \rho_q(p) = v.$$

In the thermodynamic limit on the lattice, the expectation values of the integrals of motion $\langle I_m \rangle$ are given in terms of $\rho_q(p)$ as

$$\langle I_m \rangle = M(1 - q^{-2|m|}) \frac{1}{|m|} \int_{-\pi}^{\pi} e^{-imp} \rho_q(p) dp.$$ 

If the parity symmetry is not broken, we expect $\langle I_m \rangle = \langle I_{-m} \rangle$, thus from now on we will consider only non-negative $m \geq 0$, and for convenience we introduce the notation

$$\rho_0 = \int_{-\pi}^{\pi} dp \rho_q(p) = v,$$

$$\rho_m = \frac{|m| I_m}{M(1 - q^{-2|m|})} = \int_{-\pi}^{\pi} \cos(mp) \rho_q(p) dp,$$

which are the Fourier coefficients of $\rho_q(p)$.

V. THE DENSITY $\rho_{m}(\lambda)$

A. Expectation values of the charges in the initial state

The main idea behind our regularized GGE is to use the local conserved charges of the lattice model $I_m$ to determine the $\rho_q(p)$ density of quasimomenta of $q$ bosons first, and to take the continuum limit yielding $\rho_{mLL}(\lambda)$ only as the last step.

We thus need to evaluate the expectation values of the local charges $I_m$ in a $q$-boson state which reduces to the free boson
ground state in the continuum limit (26), i.e., to the BEC state. There is no unique choice but we pick the lattice BEC state

$$|\text{BEC}_N\rangle = \frac{1}{\sqrt{N!}} \left( \frac{1}{\sqrt{M}} \sum_i b_i^\dagger \right)^N |0\rangle,$$  \hspace{1cm} (45)

where $b_i^\dagger$ are creation operators of canonical lattice bosons.

We determined the explicit expressions of the charge densities $\rho^{(m)}$ in terms of the $B_i^{(j)}$ operators up to $m = 6$. Using Eq. (28), we expand them in terms of $b_i^{(j)}$ and we normal order the result. Evaluating the expectation value in the initial state (45) amounts to a straightforward calculation with canonical lattice bosons. In this way we obtain series expansions of $\langle L_m \rangle$ in terms of the small parameter $\delta$. The details of the calculation can be found in the Appendix. We quote here only the first few terms in the expansion of the first two nontrivial charges:

$$\rho_1 = v - \frac{1}{2} \gamma v^3 + \frac{3}{16} \gamma^2 v^4 + \frac{1}{6} \gamma^2 - \frac{7}{192} \gamma^3 v^5 + \cdots,$$

$$\rho_2 = v - 2 \gamma v^3 + \frac{15}{16} \gamma^2 v^4 + \frac{5}{3} \gamma^2 - \frac{55}{192} \gamma^3 v^5 + \cdots,$$

(46)

(47)

where we use the filling fraction $v$ as a small parameter by the relation

$$\kappa = \gamma v/2,$$

(48)

which follows from Eq. (4) and the limit (26).

Naively, in the continuum limit the lattice momentum becomes small due to the relation $p = \delta \lambda$, so by combining various $\rho_m$ in Eq. (44) and Taylor expanding the integrand in terms of $p$, one could obtain moments of the $\rho_{\text{LL}}(\lambda)$ density, i.e., expectation values of the charges $\bar{Q}_m$ of the LL model. However, this must be done with care. First, the limits of integration are strictly speaking not $\pm \infty$, but $\pm \pi / \delta$, which matters if the LL moments are divergent (as expected). Second, the scaling limit (26), the relation (48) as well as the relations $\lambda = p / \delta$ and $\rho_{\text{LL}}(\lambda) = \rho_1(\delta \lambda)$ may have higher order corrections which would mix the orders.

In spite of these issues, the energy can be obtained if the $\rho_{\text{LL}}(\lambda)$ has at most a $\lambda^{-3}$ tail:

$$-\rho_1 - \rho_\lambda - 2 \rho_0 = \int_\pi -\pi dp \left( p^2 - \frac{p^4}{12} + \cdots \right) \rho_q(p)$$

$$= \int_\pi -\pi dp \lambda (\delta + \cdots) \left( \delta^2 \lambda^2 - \lambda^2 \delta^4 + \cdots \right) \langle \rho_{\text{LL}}(\lambda) + \cdots \rangle,$$  \hspace{1cm} (49)

where the dots stand for higher order terms in $\delta$. The first parentheses comes from the unknown higher order terms of the relation $p = \delta \cdot \lambda + \cdots$, this also generates terms in the middle parentheses. Now let us make the assumption that this relation, as well as the relation between $\rho_q(p)$ and $\rho_{\text{LL}}(\lambda)$, does not have higher powers of $\lambda$. Then each power $\lambda^{2n}$ comes with at least $\delta^{2n+1}$ in the integrand which implies that although the integrals of higher powers seem to diverge, with the $\delta$ powers in their coefficients all of them scale as $\delta^3$. Thus it is safe to take the $\delta \to 0$ limit after dividing by $\delta^3$ and we are left with

$$-\frac{2}{\delta^3} (\rho_1 - \rho_\lambda) \to \int_{-\infty}^{\infty} d\lambda \rho_{\text{LL}}(\lambda) \lambda^2.$$  \hspace{1cm} (50)

Since $\lim_{\delta \to 0} -\frac{2}{\delta^3}(\rho_1 - \rho_\lambda) = n^3 / \gamma$, the energy density is correctly reproduced, as expected.

In a similar fashion, one can formulate a condition on whether the $2n$th moment of the $\rho_{\text{LL}}(\lambda)$ distribution is divergent. For this one again needs to pick the right combination of $\rho_m$ with $m \leq n$. In particular, $Q_4$ is divergent if

$$\rho_2 + \rho_\lambda - 2 \rho_0 - 4 (\rho_1 + \rho_{-1} - 2 \rho_0) \propto \delta^3.$$  \hspace{1cm} (51)

From the expansion in Eqs. (A8) we find

$$\rho_2 - \rho_0 - 2 (\rho_1 - \rho_0) = \frac{3}{16} \gamma^2 n^4 \delta^4 + \cdots,$$  \hspace{1cm} (52)

thus $\int d\lambda \rho_{\text{LL}}(\lambda) \lambda^4 = (Q_4) / L$ is divergent. In the next subsection we find the exact coefficient of the corresponding $\lambda^{-4}$ tail of $\rho_{\text{LL}}(\lambda)$.

**B. Pattern for expectation values in the BEC state—large momentum expansion of $\rho_{\text{LL}}(\lambda)$**

The Taylor expansions of $\rho_m$ for $m = 1, \ldots, 6$ in terms of $\nu$ up to $O(\nu^6)$ are listed in Eqs. (A8) of the Appendix. Based on them one can find a pattern for the coefficients of the different orders. They turn out to be low order polynomials in $m$:

$$\rho_m = v - \frac{m^2}{2} \gamma v^3 + \frac{m^2 + 2 m - \frac{1}{2}}{12} \gamma^2 v^4$$

$$+ \left( \frac{m^2 (m^2 + 1)}{12} \gamma^2 - \frac{m^4 + 4m^2 - 3m + \frac{3}{2}}{96} \gamma^3 \right) v^5 + O(\nu^6).$$  \hspace{1cm} (53)

The pattern for the $O(\nu^6)$ term can be found in the Appendix. The reasonably simple rational coefficients and their structure provide strong evidence that the polynomial dependence on $m$ is correct. The order of the coefficient polynomial of $\nu^k$ is $k - 1$ and, interestingly, the subleading orders ($m^{k-2}$) are always missing. As we will show now, the first property is necessary in order to have a finite scaling limit of the $\rho_0(p)$ function, i.e., a finite $\rho_{\text{LL}}(\lambda)$.

The $\rho_0(p)$ distribution function is the Fourier sum of the $\rho_m$. It is clear that the scaling limit and this Fourier transformation do not commute: If we take the limit before computing the sum we get $\rho_m \equiv 0$. For the computation of the Fourier sum order by order in $\nu$ one needs to calculate the building blocks

$$\sum_{m=-\infty}^{\infty} m^{2l} \cos(m p) = 0,$$  \hspace{1cm} (54)

$$\sum_{m=-\infty}^{\infty} m^{2l-1} \sin(m p) = \sum_{j=0}^{l-1} c_j \cos(j p) \sin^{2l - j} \left( \frac{p}{2} \right) \rightarrow \frac{2^{2l} \sum_{j=0}^{l-1} c_j}{\delta^{2l} \lambda^{2l}},$$  \hspace{1cm} (55)

where the $c_j$ are real numbers. The second expression must be multiplied by $\delta^{2l}$ to yield neither infinity nor zero. Thus the fact that in Eq. (A10) the highest power of $m$ in the coefficient of $\nu^k$ is $k - 1$ implies that $\rho_{\text{LL}}(\lambda)$ is finite. Moreover, only the highest
powers of \( m \) in the coefficient polynomials of the even orders of \( v \) contributes. This is important, because we know the relation \( \kappa = \gamma v/2 \) only to leading order. Adding potential subleading terms \( \kappa = \gamma v/2 + a_1 v^2 + a_2 v^3 + \cdots \) generates terms in each order of \( v \) which however have a subleading \( m \) dependence, thus they do not affect the result in the continuum limit. So the results are robust against higher order corrections in \( \delta \) of the relations connecting the \( q \)-boson lattice system with the continuum LL model.

Performing the Fourier sum we obtain

\[
2\pi \rho(p) = \rho_0 + 2 \sum_{m=1}^{\infty} \rho_m \cos(mp) = v + 2 \sum_{m=1}^{\infty} \left( \frac{\gamma^2 v^4 m^3}{12} + \frac{\gamma^3 (\gamma - 24)}{960} v^6 m^5 \right) + \cdots
\]

Taking the continuum limit (26) together with \( p = \delta \lambda \) we find

\[
2\pi \rho_{\text{LL}}(\lambda) = \frac{n^2 v^2}{\lambda^2} - \frac{n^6 v^4 (\gamma - 24)}{4 \lambda^6} + \cdots. \tag{57}
\]

We see that the expansion of the Fourier modes \( \rho_m \) in terms of \( \delta \) or \( v \) is equivalent to a large momentum expansion of the LL density of roots \( \rho_{\text{LL}}(\lambda) \). We did find the expected \( \lambda^{-4} \) tail together with the subleading \( \lambda^{-6} \) tail. The coefficients of these tails in Eq. (57) are exact.

A key step in the calculation above is the rescaling of momenta \( \lambda = p/\delta \). This is how lower orders of \( v \) may eventually disappear and arbitrary high powers of \( v \) may survive in the limit. Consequently, the large momentum expansion structure can be heuristically understood by realizing that we need to resolve the vicinity of \( p = 0 \) very well, because this region will be blown up to be the entire domain in \( \lambda \). Thus it is not very surprising that many Fourier modes are necessary and one needs to know them very precisely. Any truncation or approximation affects the small \( \lambda \) region, so we approach from large \( \lambda \).

**C. Truncated GGE: Padé-Fourier approximation**

To find the full \( \rho_{\text{LL}}(\lambda) \) function one needs a pattern for the \( \rho_m \) in all orders in \( \kappa \). This requires the knowledge of the expectation values of higher charges which are increasingly hard to the compute. However, for observables of the lattice model localized on \( f \) neighboring sites the truncated GGE using the first \( m \geq 1 \) charges \( I_m \) of size \( m + 1 \) is expected to give a very good approximation.\(^{30}\) Observables localized at a point in the LL model, like \( g_k = \langle [\hat{\psi}(x)\hat{\psi}(x)]^k \rangle/n^k \), are the limits of operators localized on a few neighboring sites in the \( q \)-boson lattice system, thus we expect to capture the \( g_k \) using the first few conserved \( q \)-boson charges.

To this end, we approximate \( \rho_\lambda(p) \) by the truncated Fourier sum using the Fourier-Padé approximation. Let us consider the truncated Fourier sum,

\[
\rho_\lambda(p) = \rho_0 + 2 \sum_{m=1}^{l} \rho_m \cos(mp) = \rho_0 + 2 \sum_{m=1}^{l} \rho_m \cos(mp) = \left( \rho_0 + \sum_{m=1}^{l} \rho_m z^m \right) + [z \to 1/z], \tag{59}
\]

where we introduced \( z = e^{i\theta} \). The parenthesis is a truncated Taylor expansion to which we apply the Hermite-Padé approximation technique: We find a rational function of \( z \) such that the first \( l \) terms in its Taylor expansion matches our truncated expansion. The \((n,m)\)-type Padé approximant is a ratio of an \( n \)th order and an \( m \)th order polynomial \((n + m = l)\). We reintroduce the variable \( p \) in the approximants and then we take the continuum limit. The (2,2), (3,2), (2,3), (4,2), and (2,4) Padé approximants all give the same result,

\[
\rho_{\text{LL}}^{(1)}(\lambda) = \frac{1}{2\pi} \frac{\gamma^2}{\lambda^4 + \gamma(\gamma/4 - 2)\lambda^2 + \gamma^2}, \tag{60}
\]

where \( \bar{\lambda} = \lambda/n \). Comparing with Eq. (57) this has the correct \( \lambda^{-4} \) tail but not the \( \lambda^{-6} \) one. The latter is reproduced by the Padé approximant of type (3,3):

\[
\rho_{\text{LL}}^{(2)}(\lambda) = \frac{1}{2\pi} \frac{4\gamma^2[\bar{\lambda}^2 + \gamma(\gamma + 2)]}{(4\bar{\lambda}^2 + \gamma^2)[\bar{\lambda}^4 + (\gamma - 4)\bar{\lambda}^2 + 4\gamma^2]}. \tag{61}
\]

The densities are shown for \( \gamma = 1 \) in the inset of Fig. 1 together with the thermal grand canonical density. The latter is fixed by the energy and particle number only and is obtained by solving the standard Yang-Yang TBA equations with fixing the energy instead of the temperature. All three curves are quite different, but as we will show below, the truncated GGE solutions give nearly identical results for certain correlation functions which are different from the thermal ones.

**FIG. 1.** (Color online) Quench from a noninteracting initial state to arbitrary final interactions. **Main panel:** Local correlations \( g_2 \) and \( g_3 \) as functions of the coupling \( \gamma \), calculated from the two truncated generalized Gibbs ensembles (GGE) (red dashed, blue solid) and from the grand canonical ensemble (GCE) (dot-dashed). The asymptotic behaviors are also shown (dotted). **Inset:** Density of quasimomenta, \( \rho_{\text{LL}}^{(1)}(\lambda), \rho_{\text{LL}}^{(2)}(\lambda) \) in the two truncated GGE (red dashed, blue solid) and \( \rho_{\text{LL}}^{(h)}(\lambda) \) in the GCE (black dot-dashed) for \( \gamma = 1 \).
Let us note that, interestingly, the \( \gamma \to \infty \) limit of both \( \rho_{LL}^{(1)}(\lambda) \) and \( \rho_{LL}^{(2)}(\lambda) \) gives the Lorentzian form
\[
\lim_{\gamma \to \infty} \rho_{LL}^{(1,2)}(\lambda) = \frac{1}{2\pi} \frac{4}{(\lambda/n)^2 + 4}.
\]
This form will turn out to be the correct exact \( \rho_{LL}(\lambda) \) density for the quench to \( \gamma = \infty \).

VI. CORRELATION FUNCTIONS IN THE ASYMPOTIC STEADY STATE

A. Ultralocal observables

Knowing the density \( \rho_{LL}(\lambda) \) allows us to calculate correlation functions. First we compute point-local correlators using the results of Ref. 39 which give exact analytic expressions for the local two- and three-point correlators for arbitrary states that are captured by a continuous \( \rho_{LL}(\lambda) \). We compute
\[
g_2 = \langle \langle \hat{\psi}^\dagger \hat{\psi} \rangle^2 \rangle / n^2, \quad g_3 = \langle \langle \hat{\psi}^\dagger \hat{\psi} \rangle \langle \hat{\psi} \rangle \rangle / n^3,
\]
both for the GGE and the GCE by using the appropriate \( \rho_{LL}(\lambda) \). In the latter only the energy and the particle densities are fixed to be the same as for the GGE. The results are shown in the main panel of Fig. 1. The values of the correlators computed using the two Padé approximants are very close to each other conforming with the expectation that adding more charges to the thermal GGE does not significantly change the result. This is an important consistency check of our truncation method. The deviations are bigger for \( g_3 \) which agrees with the intuition that \( g_3 \) is more complex than \( g_2 \). The second observation is that as the difference between the two truncated results decreases for increasing \( \gamma \), their deviation from the GCE results \( g_2^{th} \) (dotted lines) grows, the relative difference between the \( g_2 \) values being bigger than 20\% for \( \gamma > 10 \). For strong interactions the asymptotic behavior of \( g_2 \) can be obtained analytically. For \( g_2 \) we find
\[
g_2 \sim \frac{8}{3\gamma}, \quad g_2^{th} \sim \frac{4}{\gamma},
\]

implying a factor of 3/2 between the two. For \( g_3 \) even the power laws are different:
\[
g_3 \sim \frac{32}{15\gamma^2}, \quad g_3^{th} \sim \frac{72}{\gamma^3}.
\]

B. Strongly interacting final state

For large coupling the system is in the fermionized Tonks-Girardeau regime since the strong repulsion induces an effective Pauli principle in real space.\(^{30}\) In the special case of the quench from \( c = 0 \) to \( c = \infty \) the overlaps between the initial state and the final TG eigenstates are explicitly known.\(^{31}\) Only states defined by a set of \( \{ \lambda_i \}_{i>0} \) have nonzero overlaps which are \( \langle \lambda_i | \text{BEC} \rangle \propto 1/\prod_{j>0} \lambda_j \). The overlaps are the necessary ingredients in the formalism of Ref. 25 to compute the saddle point density. Solving the generalized TBA equations we obtain the simple result (see also Ref. 42)
\[
\rho_{LL}(\lambda) = \frac{1}{2\pi} \frac{1}{1 + \lambda^2 n^2/4},
\]
which exactly matches the \( \gamma \to \infty \) limit of our Padé approximants [Eq. (62)]. The fact that the two derivations are completely independent gives a strong evidence for the correctness of the result.

Bosonic correlation functions can now be calculated by first fermionizing the field operators using Jordan-Wigner strings,
\[
\hat{\psi}(x) = e^\pi \int_0^{\infty} \hat{\phi}_x(z) dz \hat{\psi}_e(z),
\]
and then exploiting the free fermionic correlators of \( \hat{\psi}_e(x) \).

Let us first consider the equal time correlation \( g_2(x) = \langle \langle \hat{\psi}^\dagger(0) \hat{\psi}(x) \rangle \rangle / n \) in the saddle point distribution of Eq. (62). After introducing a lattice discretization, the long chain of operators is amenable to a Wick expansion using as a building block the fermionic two-point function. The latter is the Fourier transform of the fermionic momentum distribution which is nothing but Eq. (62) since for \( \gamma = \infty \) the quasimomenta coincide with the physical momenta. Therefore the fermionic two-point function is
\[
\langle \hat{\psi}^\dagger(0) \hat{\psi}(x) \rangle / n = e^{-2n|x|}. \]

The Wick expansion of \( \langle \hat{\psi}^\dagger(0) \hat{\psi}(0) \rangle \) can be recast as a Fredholm-like determinant\(^{43}\) that finally leads to
\[
\langle \hat{\psi}^\dagger(0) \hat{\psi}(0) \rangle / n = e^{-2n|x|}. \]

Note that this simple exponential form is exact\(^{42}\) and holds even for small \( x \). This result is drastically different from the corresponding GCE result which approaches an infinitely narrow Dirac-\( \delta \) in the TG limit. Since \( G(x) = G_{FF}(x) \), the experimentally accessible bosonic momentum distribution \( n_B(k) \) is equal to the Lorentzian \( \rho_{LL}(k) \) given by Eq. (62), plotted in the inset of Fig. 2.

We can also compute the density-density correlation function
\[
g_2(x) = \langle \langle \hat{\psi}^\dagger(0) \hat{\psi}(0) \hat{\psi}(x) \rangle \rangle / n^2
\]
for large final \( \gamma \) using the first few terms of the infinite series given in Ref. 44. In the large \( \gamma \) limit the leading order for arbitrary \( \rho(\lambda) \) is given by \( g_2(x) \approx 1 - [\int d\lambda \rho(\lambda) e^{i\lambda x}]^2 \). Using
\[ g_2(x) = 1 - e^{-4|x|}, \tag{71} \]

which agrees very well with the large time result of the numerical solution of the time evolution in Ref. 41 based on the exact overlaps (see main panel of Fig. 2). To the best of our knowledge this is one of the first demonstrations in a continuum integrable model that the GGE value of an observable agrees with its actual large time asymptotics.

VII. CONCLUSIONS

Extending the studies of the post-quench behavior of many-body systems to a nonquadratic continuum model, we investigated the large time behavior of the Lieb-Liniger model after an interaction quench using analytic techniques by combining the generalized Gibbs ensemble and Bethe ansatz integrability of the model and its lattice discretization. We pointed out the divergence of local charges in the initial state that prevents the naive application of the GGE ansatz integrability of the model and its lattice discretization. We expect this to be a generic phenomenon for interaction quenches in continuum models with contact interactions which deserves further study. For a noninteracting initial state and arbitrary final interactions, we evaluated local correlations and found deviations from the thermal predictions. These are experimentally accessible through the measurement of the photoassociation rate \((g_2)\) and the inelastic three-body loss \((g_3)\) in cold atom experiments. We computed two-point correlation functions exactly for quenches to the fermionized Tonks-Girardeau regime and found excellent agreement with a recent numerical simulation of the time evolution.

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APPENDIX

In the Appendix we give some details about the calculation of expectation values in the initial lattice BEC state,

\[ |\text{BEC}\rangle_N = \frac{1}{\sqrt{N!}} \left( \frac{1}{\sqrt{M}} \sum_i b_i \right)^N |0\rangle. \tag{A1} \]

This state has the nice property (established by commuting annihilation operators one by one)

\[ b_j^\dagger |\text{BEC}\rangle_N = \sqrt{\frac{N}{M}} \cdots \sqrt{\frac{N - \alpha + 1}{M}} |\text{BEC}\rangle_{N-\alpha} \approx \nu^{\alpha/2} |\text{BEC}\rangle_{N-\alpha}, \tag{A2} \]

where the approximate relation is valid in the thermodynamic limit when we are interested in \(\alpha\) that does not scale proportionally to the system size. Note that as long as we are interested in the evaluation of expectation values of normal ordered operators over BEC state in the TDL, one can also use the coherent state form of the BEC,

\[ |\text{BEC},c\rangle = \prod_j e^{-\nu^2/2 + \nu^2 b_j^\dagger} |0\rangle, \tag{A3} \]

which has the same matrix elements as the state (A2).

In what follows, we compute expectation values of the local charges by computing first the building blocks, on-site monomials, based on expanding \(B_j^{(1)}\) in terms of \(b_j^{(1)}\) and normal ordering. For most of the matrix elements we can only derive expansions in powers of \(\kappa\) (but not making any assumptions about \(v\)). We will start from

\[ B_j = bj\sqrt{\frac{(N + 1)j}{N + 1}} \approx bj \left( 1 - \frac{\kappa}{2N}j + \frac{\kappa^2}{24}N(j(5N + 4) + \cdots) \right) = bj - \frac{\kappa}{2}b_j^\dagger b_j b_j + \frac{\kappa^2}{24}(5b_j^\dagger b_j b_j + bj b_j b_j + 9b_j^\dagger b_j b_j) + \cdots \tag{A4} \]

The evaluation of its expectation value in the state (A3) leads to

\[ \langle \text{BEC},c | B_j | \text{BEC},c \rangle = \sqrt{\nu} - \frac{1}{2}\kappa\nu^{3/2} + \frac{\kappa^2}{24}(9\nu^{3/2} + 5\nu^{5/2}) + \cdots . \tag{A5} \]

In a similar way we obtain

\[ \langle \text{BEC} | B_j^\dagger B_j | \text{BEC} \rangle = \nu - \kappa\nu^2 + \frac{\kappa^2}{24}\nu^3 + \frac{\kappa^2}{24}\nu^{5/2} + \cdots . \tag{A6} \]

We note that for this combination a closed form expression exists, \(\langle \text{BEC} | B_j^\dagger B_j | \text{BEC} \rangle = (1 - e^{-(1-\nu^2)\kappa})/(1 - q^2)\). These and similar on-site matrix elements are the only type needed to systematically evaluate the expectation values of any polynomial of
B\(^{(1)}\) operators acting on different sites over the BEC. Indeed, due to the factorization of the wave function on different sites in the coherent state representation (A3) one can treat different sites separately. Let us now use these matrix elements to evaluate the first \(\rho_m, m = 1, \ldots, 6\). From Eqs. (34) and (35) and from the definition (44) we have

\[
\rho_1 = \frac{1}{M} \sum_j (B_j^\dagger B_{j+1}), \quad \rho_2 = \frac{1}{M} \sum_j \left( B_j^\dagger B_{j+2} - \frac{\chi^2}{2 - \chi^2} B_j^\dagger B_j B_{j+1} B_{j+2} - \chi^2 B_j^\dagger B_{j+1} B_{j+2} \right), \text{ etc.}
\]

Due to translational invariance we need to evaluate the expectation value only for a single value of \(j\). We find

\[
\rho_1 = v - \frac{1}{2} \gamma v^3 + \frac{3}{16} \gamma^2 v^4 + \left( \frac{1}{6} \gamma^2 - \frac{7}{192} \gamma^3 \right) v^5 - \frac{11}{96} \gamma^3 v^6 + \ldots,
\]

\[
\rho_2 = v - 2 \gamma v^3 + \frac{15}{16} \gamma^2 v^4 + \left( \frac{5}{3} \gamma^2 - \frac{55}{192} \gamma^3 \right) v^5 + \left( \frac{51}{32} \gamma^3 + \frac{1}{16} \gamma^4 \right) v^6 + \ldots,
\]

\[
\rho_3 = v - \frac{9}{2} \gamma v^3 + \frac{43}{16} \gamma^2 v^4 + \left( \frac{15}{8} \gamma^2 - \frac{73}{64} \gamma^3 \right) v^5 + \left( \frac{859}{96} \gamma^3 + \frac{73}{192} \gamma^4 \right) v^6 + \ldots,
\]

\[
\rho_4 = v - 8 \gamma v^3 + \frac{95}{16} \gamma^2 v^4 + \left( \frac{68}{12} \gamma^2 - \frac{419}{192} \gamma^3 \right) v^5 + \left( \frac{3137}{96} \gamma^3 + \frac{269}{192} \gamma^4 \right) v^6 + \ldots,
\]

\[
\rho_5 = v - \frac{25}{2} \gamma v^3 + \frac{179}{16} \gamma^2 v^4 + \left( \frac{325}{6} \gamma^2 - \frac{1423}{192} \gamma^3 \right) v^5 + \left( \frac{2953}{32} \gamma^3 + \frac{379}{96} \gamma^4 \right) v^6 + \ldots,
\]

\[
\rho_6 = v - 18 \gamma v^3 + \frac{303}{16} \gamma^2 v^4 + \left( \frac{111}{2} \gamma^2 - \frac{649}{64} \gamma^3 \right) v^5 + \left( \frac{21049}{96} \gamma^3 + \frac{299}{32} \gamma^4 \right) v^6 + \ldots,
\]

where we use \(\nu\) as small parameter by the relation

\[
\kappa = \gamma \nu / 2.
\]

One can conjecture the pattern for the coefficients of the different orders. They turn out to be low order polynomials in \(m\):

\[
\rho_m = v - \frac{m^2}{2} \gamma v^3 + \frac{m^3 + 2m - 3}{12} \gamma^2 v^4 + \left( \frac{m^2 (m^3 + 1)}{12} \gamma^2 - \frac{m^4 + 3m^2 - m + 3}{96} \gamma^3 \right) v^5
\]

\[
+ \left( - \frac{m^5 + 5m^3 - 5}{40} m^2 + \frac{5}{2} m + \frac{5}{12} \gamma^3 + \frac{m^5 + 20}{3} m^3 - \frac{15}{2} m^2 + \frac{29}{6} m - \frac{5}{4} \right) \gamma^4 v^6 + O(\gamma^7).
\]

\(^2\)kormos@eik.bme.hu
\(^3\)Deceased.


19. I. Mossel (private communication).


