Complete Generalized Gibbs Ensembles in an Interacting Theory

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In this Letter, we settle this issue by explicitly showing how to repair the GGE in Heisenberg chains, by complementing it with recently discovered additional families of conserved charges [31]. Crucially, these “quasilocal” charges fulfill a weaker form of locality than the previously known ones. We derive a set of fundamental identities between the initial-state expectation values of these charges, and the density functions characterizing the steady state. An explicit test of our construction is provided by a quantum quench from the Néel state to the XXZ chain: we

Introduction.—Understanding and describing the equilibration of isolated many-particle systems is one of the main current challenges of quantum physics. The presence of higher conserved charges (above the Hamiltonian) is linked to the absence of full relaxation to a thermalized state; the conjectured appropriate framework to characterize the steady-state properties in such a situation is the generalized Gibbs ensemble (GGE) [1], in which all available charges are ascribed an individual “chemical potential” set by the initial conditions, and the steady state is the maximal entropy state fulfilling all the constraints associated to the conserved charges [2–27]. The basic idea underlying the GGE is as follows. Let \( H = H^{(1)} \) be the Hamiltonian of an integrable model, and \( \{H^{(n)}\} \) a set of conserved charges fulfilling \( [H^{(n)}, H^{(m)}] = 0 \). The situation we are interested in is that of a quantum quench, where we initially prepare our system in the ground state \( |\Psi(0)\rangle \) of a local Hamiltonian \( H_0 \) and then consider unitary time evolution with respect to our integrable Hamiltonian

\[
|\Psi(t)\rangle = e^{-iHt}|\Psi(0)\rangle.
\]

We assume that we are dealing with a generic case where, in the thermodynamic limit, \( |\Psi(0)\rangle \) cannot be expressed as a linear combination of any finite number of eigenstates of \( H \). At late times after the quench expectation values of local operators approach stationary values

\[
\langle O \rangle_\Psi = \lim_{t \to \infty} \langle \Psi(t)|O|\Psi(t)\rangle.
\]

The GGE hypothesis asserts that these expectation values can be calculated as \( \langle O \rangle_\Psi = \text{Tr}(\hat{\rho}_{\text{GGE}} O) \) from a statistical ensemble with a density matrix

\[
\hat{\rho}_{\text{GGE}} = \frac{1}{Z} \exp \left[-\sum_n \beta_n H^{(n)}\right].
\]

Here \( Z \) is a normalization, and the Lagrange multipliers \( \beta_n \) are fixed by the initial conditions

\[
\lim_{t \to \infty} \frac{\text{Tr}(\hat{\rho}_{\text{GGE}} H^{(n)})}{N} = \lim_{t \to \infty} \frac{\langle \Psi(0)|H^{(n)}|\Psi(0)\rangle}{N},
\]

where \( N \) is the system size and \( \lim_{t \to \infty} \) denotes the thermodynamic limit \( N \to \infty \). Equation (4) is a direct consequence of the fact that \( H^{(n)} \) are conserved charges. While the GGE hypothesis has been successfully verified for many systems mappable to free particles, in interacting theories such as the spin-1/2 Heisenberg XXZ chain the question of precisely which charges need to be included in Eq. (3) arises. In Refs. [17,18,20] a GGE based on the known conserved local charges [28] was constructed and used to determine steady-state averages of observables [20]. Subsequent analyses [21,22] by the Quench Action (QA) approach [14] demonstrated that this GGE fails to predict the correct steady-state properties. This failure was shown to be related to the existence of bound states [21] (see also [29,30]), which are known to be a generic feature in quantum integrable models. These results posed the question of whether the GGE is conceptually faulty, or whether there could exist hitherto unknown charges that need to be taken into account in its construction.

In this Letter, we settle this issue by explicitly showing how to repair the GGE in Heisenberg chains, by complementing it with recently discovered additional families of conserved charges [31]. Crucially, these “quasilocal” charges fulfill a weaker form of locality than the previously known ones. We derive a set of fundamental identities between the initial-state expectation values of these charges, and the density functions characterizing the steady state. An explicit test of our construction is provided by a quantum quench from the Néel state to the XXZ chain: we
demonstrate that our GGE correctly recovers the stationary state, the form of which is known exactly from the QA approach [21,32]. In this way we completely resolve the above-mentioned conundrum. Our construction shows that quasilocal conserved charges are in fact crucial for understanding the nonequilibrium dynamics of quantum integrable models.

Anisotropic spin-1/2 Heisenberg chain.—We shall consider a completely generic quench protocol from an initial pure wave function |Ψ0⟩, which is unitarily time evolved according to the Hamiltonian

\[ H = \frac{J}{\lambda} \sum_{j=1}^{N} [\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta(\sigma_j^z \sigma_{j+1}^z - 1)]. \]  

(5)

Here \( J > 0 \), \( \sigma_j^a \), \( a = x,y,z \) are Pauli matrices acting on spin-1/2 degrees of freedom, and we consider anisotropy values in the regime, \( \Delta = \cot \theta \geq 1 \). The Hamiltonian given by Eq. (5) can be diagonalized by Bethe Ansatz [33,34].

Imposing periodic boundary conditions, energy eigenstates |λ⟩ with magnetization \( S_{zz}^i = N/2 - M \) are labeled by a set of rapidities \( λ = \{ λ_i \}^{M}_{i=1} \) satisfying the Bethe equations,

\[ \sin(\lambda_j + i n/2)/\sin(\lambda_j - i n/2)]^N = -\prod_{k=1}^{M} \sin(\lambda_j - \lambda_k + i n)/\sin(\lambda_j - \lambda_k - i n), \]  

where \( j = 1, ..., M \). The momentum and energy of a Bethe state are \( p_λ = \sum_{j=1}^{M} p(λ_j), \; ω_λ = \sum_{j=1}^{M} e(λ_j), \) where \( p(λ) = i \ln(\sin(\lambda - i n/2)/\sin(\lambda + i n/2)) \) and \( e(λ) = -Jπ \sinh(n) a_1(λ) \), where

\[ a_n(λ) = \frac{2 \sinh(n\eta)}{2π \cosh(n\eta) - \cos(2λ)}. \]  

(6)

Solutions \( λ \) to the Bethe equations are closed under complex conjugation and consist of so-called strings \( \lambda_a^{n,a} = λ_a^n + \frac{π}{2}(n + 1 - 2a) + iδ_{a}^n, \; a = 1, ..., n \), and \( λ_a^n ∈ \mathbb{R} \). Here index \( a \) enumerates a string, \( n \) is the string length, \( a \) counts rapidities inside a given string, and deviations \( δ_a^n \) are (for the majority of states) exponentially small in system size [28,35,36]. The string centers \( λ_a^n \) lie in the interval, \( [-π/2, π/2] \). In the thermodynamic limit \( N \to ∞ \) with \( M/N \) fixed, one can describe a state not in terms of individual rapidities, but rather in terms of a set of functions \( ρ = \{ ρ_n \}_{n=1}^{∞} \) representing string densities (see Supplemental Material for more info [37]).

Ultralocal GGE treatment.—Exactly solvable Hamiltonians such as Eq. (5) can be embedded [28] in a commuting family \([T(λ), T(λ')] = 0\) of transfer matrices [defined in Eq. (15)]. The Hamiltonian and an infinite number of mutually commuting conserved charges are obtained by

\[ H^{(n)} = \frac{i}{n!} ∂_λ^n \log T(-iλ)|_{λ=0}. \]  

(7)

with the Hamiltonian reading \( H = \frac{J \sinh(n\eta)}{2} H^{(1)} \). These charges are ultralocal in the sense that they can be written as \( H^{(n)} = \sum_{j=1}^{N} h_j^{(m)} \), where the operators \( h_j^{(m)} \) act nontrivially on a block of at most \( m \) sites adjacent to \( j \). The GGE constructed in [17,18] was of the form given by Eqs. (3) and (4), with charges from Eq. (7). The initial values \( h^{(n)} = \lim_n N^{-1} ⟨Ψ(0)|H^{(n)}|Ψ(0)⟩ \) of the conserved charges are conveniently encoded in the generating function [18]

\[ \Omega^{ψ}_0(λ) = \lim \frac{i}{N} ⟨Ψ_0|T^{-1}(λ + iη/2) ∂_λ T(λ + iη/2)|Ψ_0⟩ \]  

\[ = \sum_{k=0}^{∞} \frac{λ^k}{k!} h(k+1). \]  

(8)

Given the GGE density matrix, a “microcanonical” description of the steady state can be obtained by performing a generalized Thermodynamic Bethe Ansatz [11,38]; see Supplemental Material for a brief summary [37]. This results in a representative eigenstate |ψ_GGE⟩ labeled by root density functions \( ρ_ρ \), which has the property that for any local operator \( C \),

\[ Tr(C|ψ_GGE⟩) = ⟨ρ_GGE|C|ψ_GGE⟩. \]  

(9)

Within the generalized Thermodynamic Bethe Ansatz formalism macrostates can be described either by root densities of particles, or by densities of holes. Holes can be, loosely speaking, understood as analogues of unoccupied states in models of free fermions. In terms of the latter the state |ψ_GGE⟩ is parametrized in terms of the set of positive functions \( \{ ρ^{ψ}_0 \}_{n,h} \). In [21,32] it was found that the initial data, Eq. (4), directly determines the hole density of 1-strings (i.e., vacancies of unbound states), according to the remarkable identity

\[ ρ^{ψ}_0(λ) = a_1(λ) + \frac{1}{2π} \left[ \Omega^{ψ}_0(λ + iη/2) + Ω^{ψ}_0(λ - iη/2) \right]. \]  

(10)

All other hole densities are fixed by the maximum entropy principle under the constraints of Eq. (4).

Quench action treatment.—The above GGE treatment should be compared to an independent calculation using the QA method [14]. For a generic quench problem, given an initial state |ψ_0⟩, the time-dependent expectation value of a generic local observable \( O \) can be expressed as a double Hilbert space summation

\[ ⟨Ψ(t)|O|Ψ(t)⟩ = \sum_{λ,λ'} e^{−S_{λ−λ'}} e^{i(a_1(λ)−a_1(λ'))} ⟨λ|O|λ'⟩. \]  

(11)

where \( S_{λ} = −\ln ⟨λ|ψ_0⟩ \). Here, |λ⟩ are eigenstates of the Hamiltonian driving the postquench time evolution. Exploiting the fact that in the thermodynamic limit, the summation over eigenstates can be written as a functional integral over root densities, which can be evaluated in a saddle-point approximation (becoming exact in the thermodynamic limit), one finds, in particular, that the steady-state
expectation values of observables a long time after the quench can be obtained as
\[
\lim_{t \to \infty} \lim_{n \to \infty} \langle \Psi(t) | \mathcal{O} | \Psi(t) \rangle = \langle \rho_{QA}^{\psi_0} | \mathcal{O} | \rho_{QA}^{\psi_0} \rangle.
\]  
(12)

Here $| \rho_{QA}^{\psi_0} \rangle$ is an eigenstate minimizing the QA $S_{QA}[\rho] = 2S[\rho] - S_{YY}[\rho]$, where $S[\rho] = \lim_q \text{ReS}_q$ is the extensive real part of the overlap coefficient in the thermodynamic limit and $S_{YY}[\rho]$ is the Yang-Yang entropy of the state $[28,35,36]$. For the Néel to XXZ quench, the exact overlaps were obtained in [39] and used in [21,32] to obtain the exact saddle-point densities $\rho_{QA}^{\psi_0}$ representing the steady state. Crucially, one finds [21,22] that $\rho_{GGE}^{\psi_0} \neq \rho_{QA}^{\psi_0}$, which in turn leads to different predictions for physical properties such as spin-spin correlators. This demonstrated that the ultralocal GGE does not correctly describe the steady state after a generic quantum quench in the XXZ chain.

Constructing a quasilocal GGE.—Very recently [31] (see also [40–45]) hitherto unknown conserved charges of the isotropic ($\Delta = 1$) Heisenberg model were discovered. These operators are not local in the sense that they cannot be represented as a spatially homogeneous sum of finitely supported densities, but rather quasilocal, meaning [31] that their Hilbert–Schmidt norms scale linearly with system size and their overlaps with locally supported operators become independent of $N$ in the limit of large system size. Moreover, they are linearly independent from the known local charges generated from the spin-1/2 transfer matrix. Until now, the impact of these charges on local physical observables has not been quantified.

Our first step is to construct a family of quasilocal conserved charges for $\Delta \geq 1$ by generalizing the procedure of [31]. The starting point is the $q$-deformed $L$-operator,
\[
L(z,s) = \frac{1}{\sinh(\eta)} \left[ \sinh(z) \cosh(qs^2) \otimes \sigma^0 + \cosh(z) \sinh(qs^2) \otimes \sigma^z + \sinh(\eta)(s^- \otimes \sigma^+ + s^+ \otimes \sigma^-) \right],
\]

(13)

whose auxiliary-space components are given by $q$-deformed spin-$s$ representations with $s = \frac{1}{2}, 1, \frac{3}{2}, \ldots$, obeying commutation relations $[s^+, s^-] = [2s^2]_q, [s^z, s^\pm] = \pm s^\pm$ and acting in a $(2s + 1)$-dimensional irreducible representation, $\mathcal{V}_s \cong \mathbb{C}^{2s+1} = \text{Isp}\{[k]; k = -s, \ldots, s\}$,
\[
s^+|k\rangle = k|k\rangle, \quad s^-|k\rangle = \sqrt{[s + 1 \pm k]_q[s \mp k]_q}|k \pm 1\rangle,
\]

(14)

where $[x]_q = \sinh(\eta x)/\sinh(\eta)$. By means of higher-spin auxiliary (fused) transfer matrices defined via ordered products of $L$-operators
\[
T_s(z) = \text{Tr}_{\mathcal{V}_s} [L_{a,1}(z,s) \ldots L_{a,N}(z,s)],
\]

(15)

[where $T_{1/2}(z) \equiv T(z)$ was used in Eq. (7)] we define families of conserved operators $X_s(\lambda) = \tau_s^{-1}(\lambda) \{ T_s(z^\pm_{\lambda}) T_s(z^\mp_{\lambda}) \}$. With $T_s(z) = \partial_z T_s(z)$ and $\{ \star \}$ denoting the traceless part. The normalization reads $\tau_s(\lambda) = f[-(s + 1 \eta) + i\lambda] \times f[(s + 1 \eta) + i\lambda]$ with $f(z) = [\sinh(z)/\sinh(\eta)]^{\eta}$. In [31] it was shown for the isotropic case that these charges are quasilocal for all $s = \frac{1}{2}, 1, \frac{3}{2}, \ldots, \lambda \in \mathbb{R}$. A rigorous proof for general $\Delta > 1$ is currently under construction [46].

A central piece of our work is the extraction of the thermodynamically leading part of the quasilocal charges $\{X_s\}_{s=1/2}^\infty$ when operating on an arbitrary Bethe state. It proves useful to resort to the so-called fusion relations [47–50] ($T$-system) for higher-spin transfer matrices,
\[
T_s \left( z + \frac{\eta}{2} \right) T_s \left( z - \frac{\eta}{2} \right) = f \left[ z + \left( s + \frac{1}{2} \right) \eta \right] f \left[ z - \left( s + \frac{1}{2} \right) \eta \right] + T_{s-1/2}(z) T_{s+1/2}(z),
\]

(17)

with the initial condition $T_0(z) \equiv f(z)$. There exists a closed-form solution to the above recurrence relation in terms of Baxter’s $Q$-operators [48]
\[
T_s(z) = Q \left[ z + \left( s + \frac{1}{2} \right) \eta \right] Q \left[ z - \left( s + \frac{1}{2} \right) \eta \right] \times \sum_{\ell=0}^{2s} f[\ell + (\ell - s)\eta] Q[z + (\ell - s + \frac{1}{2})\eta],
\]

(18)

The eigenvalues of the $Q$-operators [in what follows, in view of commutations $[T_s(z_1), Q(z_2)] = 0, \forall s, z_i \in \mathbb{C}$, we slightly abuse notation by using the same symbol for an operator and its eigenvalue] are determined by the position of Bethe roots, $Q(z) = \prod_{k=1}^{d_s} \sinh(z + i\lambda_k)$. A key observation is that, in the thermodynamic limit, the spin-$s$ transfer matrix evaluated at $z^+_s$ ($z^-_s$) is simply given by $\ell = 0$ ($\ell = 2s$) term in the sum in Eq. (18). This then gives
\[
\lim_{\text{th}} T_s(z^\pm_{\lambda}) = \lim_{\text{th}} f \left[ \pm \left( s + \frac{1}{2} \right) \eta + i\lambda \right] Q[\mp s\eta + i\lambda].
\]

(19)

The latter analysis is consistent with $\lim_{\text{th}} \tau_s^{-1}(\lambda) \{ T_s(z^\pm_{\lambda}) \} \times T_s(z^\mp_{\lambda}) = 1$, representing a thermodynamic version of an inversion identity (see [31]) that can be proven in an entirely operatorial way, without making reference to the Bethe eigenstates. At this point it is convenient to define modified conserved operators
\[
\hat{X}_s(\lambda) = T_s^{-1}(z^-_{\lambda}) T_s^{(s)}(z^+_{\lambda}),
\]

(20)

where $T_s^{(s)}(z)$ have the same structure as in Eq. (15) but involve $L$-operators, $L^{(s)}(z,s) = L(z,s) \sinh(\eta)/[\sinh(z \pm s\eta)]$. In the thermodynamic limit a quasilocal conserved operator
\( \hat{X}_s(\lambda) \) only differs from \( X_s(\lambda) \) by a multiple of identity, 
\( \hat{X}_s(\lambda) = X_s(\lambda) + t_s(\lambda) \mathbb{1} \), with 
\( t_s(\lambda) = [2s/(2s + 1)] \times \{ \sinh [(2s + 1)\eta]/[\sinh^2(\eta)] \} \xi_s^{-1}(\lambda) \). We can now define a two-parameter family of conserved charges

\[
H^{(n)}_s = \frac{1}{n!} \partial^n \hat{X}_s(\lambda) |_{\lambda = 0}.
\]

By construction we have \([H^{(n)}_s, H^{(m)}_{s'}] = 0 \) and \( \{H^{(n)}_s\}_n \) precisely recover the ultralocal conservation laws from Eq. (7). We are thus in a position to define the density matrix of our GGE. It is given by

\[
\hat{\rho}_{\text{GGE}} = \frac{1}{Z} \exp \left[ - \sum_{n,k=1}^{\infty} \beta_n \hat{H}^{(n)}_{s/2} \right],
\]

where the Lagrange multipliers \( \beta_n \) are fixed by initial conditions given by Eq. (4). Our assertion is that Eq. (22) provides a correct description of the stationary behavior after a general quench to the spin-1/2 XXZ chain (in the regime \( \Delta \geq 1 \)). In order to prove this it suffices to establish that the initial values of our conserved charges uniquely specify a macrostate.

Let us now derive the main result of our Letter. Analogously to what was found in [21,32] for the ultralocal charges, the values of the quasilocal charges associated with a spin-\( s \) transfer matrix are in one-to-one correspondence with functions \( \rho^{(s)}_{2s,2s}(\lambda) \), which in turn specify (see Supplemental Material [37]) a unique macrostate (namely, the GGE saddle-point state).

Our starting point is the following expression for the spectrum of \( \{ \hat{X}_s \}_s \), valid for the large system size [cf. Eq. (19)]:

\[
\hat{X}_s(\lambda) = -i \partial \log \frac{Q(-s\eta + i\lambda)}{Q(s\eta + i\lambda)} + o(N)
\]

\[= \sum_{k=1}^{M} \frac{\sinh(2s\eta)}{\cos[2(\lambda_k + \lambda)] - \cosh(2s\eta)} + o(N). \tag{23}\]

Starting from Eq. (23), working in the thermodynamic limit under the string hypothesis and making use of Bethe equations, one arrives at (see Supplemental Material [37])

\[
\rho^{(s)}_{2s,2s}(\lambda) = a_{2s}(\lambda) + \frac{1}{2\pi} \Omega^{(s)}(\lambda + \frac{i\eta}{2}) + \Omega^{(s)}(\lambda - \frac{i\eta}{2}), \tag{24}\]

where \( s = \frac{1}{2}, 1, \frac{3}{2}, \ldots \). The right-hand side of Eq. (24) is determined by the expectation values of the quasilocal charges on the initial state,

\[
\Omega^{(s)}(\lambda) = \lim_{n \to \infty} \frac{\langle \Psi_0 | \hat{X}_s(\lambda) | \Psi_0 \rangle}{N}. \tag{25}\]

This is a generalization of Eq. (10) to arbitrary spin. Note the remarkable fact that this correspondence is valid for a generic initial state \( |\Psi_0 \rangle \). As a consequence, the family of quasilocal charges \( \{ \hat{X}_s \}_s \) completely determines the postquench stationary state through the GGE and gives the latter's predictions identical to those coming from the QA.

\subsection*{Néel quench.}

An explicit example of our construction is provided by the quench from the Néel state

\[
|\Psi_0 \rangle = \frac{1}{\sqrt{2}} (|\uparrow \downarrow \uparrow \downarrow \cdots \rangle + |\downarrow \uparrow \downarrow \uparrow \cdots \rangle). \tag{26}\]

Here the root distributions characterizing the stationary state have been previously determined by a QA calculation [21,32]. In order to demonstrate that our GGE recovers these known results we need to compute the generating functions, Eq. (25). Here we can repeat the logical steps from the calculation for \( s = 1/2 \) in [18,20] by studying the spectrum of associated auxiliary transfer matrices. This calculation can be found in the Supplemental Material [37]. Substituting the results obtained in this way into Eq. (24) gives perfect agreement with the known QA results.

\subsection*{Towards a truncated GGE.}

In [10] it was argued that for the purpose of describing finite subsystems in the thermodynamic limit ultralocal GGEs can be truncated by retaining only a finite number of the “most local” conserved charges. An obvious question is whether a similar logic can be applied to our quasilocal GGE. As a first step towards understanding this issue, we have calculated the next-nearest spin correlation function in the steady state after a Néel-to-XXZ quench for several GGE truncations in the \( s \) direction. In Fig. 1 we show the results of these calculations for \( \Delta \geq 1 \). The data clearly show that adding subsequent families of quasilocal charges results in a rapid convergence of the corresponding truncated GGE result to the exact value.

\subsection*{Conclusions.}

We have shown how to construct an exact GGE describing the stationary state after generic quantum quenches to the spin-1/2 Heisenberg XXZ chain. Our GGE is built from an extended set of local and quasilocal charges. We have shown that our construction resolves
previously observed discrepancies between predictions for steady-state expectation values by an exact QA treatment on the one hand, and a GGE restricted to ultralocal charges obtained from the transfer matrix of the spin-$1/2$ chain on the other hand. Our results provide unambiguous proof that the recently discovered quasilocal charges have a non-negligible impact on the relaxation processes of strongly interacting many-body quantum systems in one dimension.

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[37] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.115.157201 for technical details on the Thermodynamic Bethe Ansatz equations and generalizations thereof involving descriptions for the GGE and Quench Action methods, a derivation of an explicit relation between hole distributions and generating functions for quasi-local charges, a short explanation on the implementation of the truncated GGE as shown in Fig 1, and details on the computation of generating functions for a particular problem of the Neeq quench.

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