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Published in:
Physical Review Letters

DOI:
10.1103/PhysRevLett.115.157201

Citation for published version (APA):

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Complete Generalized Gibbs Ensembles in an Interacting Theory

E. Ilievski,1 J. De Nardis,1 B. Wouters,1 J.-S. Caux,1 F. H. L. Essler,2 and T. Prosen3

1Institute for Theoretical Physics, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands
2The Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3NP, United Kingdom
3Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, SI-1000 Ljubljana, Slovenia

(Received 21 July 2015; published 7 October 2015)

In integrable many-particle systems, it is widely believed that the stationary state reached at late times after a quantum quench can be described by a generalized Gibbs ensemble (GGE) constructed from their extensive number of conserved charges. A crucial issue is then to identify a complete set of these charges, enabling the GGE to provide exact steady-state predictions. Here we solve this long-standing problem for the case of the spin-1/2 Heisenberg chain by explicitly constructing a GGE which uniquely fixes the macrostate describing the stationary behavior after a general quantum quench. A crucial ingredient in our method, which readily generalizes to other integrable models, are recently discovered quasilocal charges. As a test, we reproduce the exact postquench steady state of the Néel quench problem obtained previously by means of the Quench Action method.

DOI: 10.1103/PhysRevLett.115.157201

PACS numbers: 75.10.Jm, 02.30.Ik, 05.30.-d, 05.70.Ln

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

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

The GGE hypothesis asserts that these expectation values can be calculated as $\langle \mathcal{O} \rangle_\Psi = \text{Tr}(\hat{\rho}_{\text{GGE}} \mathcal{O})$ 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
describe a state not in terms of individual rapidities, but rather
\[ H = J \sum_{j=1}^{N} \left[ \sigma^x_j \sigma^x_{j+1} + \sigma^y_j \sigma^y_{j+1} + \Delta (\sigma^z_j \sigma^z_{j+1} - 1) \right]. \]

Here \( J > 0, \sigma^a_j, a = x, y, z \) are Pauli matrices acting on spin-1/2 degrees of freedom, and we consider anisotropy
values in the regime, \( \Delta = \cosh(\eta) \geq 1 \). The Hamiltonian
given by Eq. (5) can be diagonalized by Bethe Ansatz \[33,34\].
Imposing periodic boundary conditions, energy eigenstates
\( |\lambda\rangle \) with magnetization \( S^z_{\text{tot}} = N/2 - M \) are labeled by a
set of rapidities \( \lambda = \{ \lambda_k \}_{k=1}^{M} \) satisfying the Bethe equations,
\[ \sin(\lambda_j + i\eta/2)/\sin(\lambda_j - i\eta/2) = \frac{\prod_{k=1}^{M} (\sin(\lambda_j - \lambda_k + i\eta)/ \sin(\lambda_j - \lambda_k - i\eta))}{\prod_{k=1}^{M} (\sin(\lambda_j + \lambda_k + i\eta)/ \sin(\lambda_j + \lambda_k - i\eta))}, \quad j = 1, \ldots, M. \]
The momentum and energy
of a Bethe state are
\[ P_k = \sum_{j=1}^{M} p(\lambda_j), \quad \omega_k = \sum_{j=1}^{M} e(\lambda_j), \]
where
\[ p(\lambda) = i \ln \left( \frac{\sin(\lambda - i\eta/2)}{\sin(\lambda + i\eta/2)} \right) \]
\[ e(\lambda) = -J \pi \sinh(\eta) a_1(\lambda), \]
and
\[ a_n(\lambda) = \frac{1}{2\pi} \frac{2 \sinh(n\eta)}{\cosh(n\eta) - \cos(2\lambda)}. \]

Solutions \( \lambda \) to the Bethe equations are closed under complex
conjugation and consist of so-called strings \( \lambda^a_{n\alpha} = \lambda_n^a + \frac{\pi}{2} (n + 1 - 2\alpha) + i\Theta^a_n, \alpha = 1, \ldots, n \), and \( \lambda^a_{n\alpha} \in \mathbb{R} \). Here index
\( \alpha \) enumerates a string, \( n \) is the string length, \( \Theta^a \) counts rapidities
inside a given string, and deviations \( \Theta^a_n \) are (for the majority of
states) exponentially small in system size \[28,35,36\]. The
string centers \( \lambda^a_n \) lie in the interval, \( [-\pi/2, \pi/2] \). In the
thermodynamic limit \( N \to \infty \) with \( M/N \) fixed, one can describe a state not in terms of individual rapidities, but rather
in terms of a set of functions \( \rho = \{ \rho_n \}_{n=1}^{\infty} \) representing string
densities (see Supplemental Material for more info \[37\]).

**Anisotropic spin-1/2 Heisenberg chain.**—We shall consider a completely generic quench protocol from an initial
pure wave function \( |\Psi_0\rangle \), which is unitarily time evolved
according to the Hamiltonian
\[ \Omega^{Q_0}(\lambda) = \lim_{\eta \to 0} \frac{i}{N} \langle \Psi_0 | T^{-1} \left( \lambda + \frac{i\eta}{2} \right) \partial_\lambda T \left( \lambda + \frac{i\eta}{2} \right) |\Psi_0\rangle \]
\[ = \sum_{k=0}^{\infty} \frac{\lambda^k}{k!} h^{(k+1)}(\lambda). \]

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 \( |\Psi_{GGE}\rangle \)
with the property that for any local operator \( \mathcal{O} \),
\[ \text{Tr}(\mathcal{O} |\Psi_{GGE}\rangle) = \langle \mathcal{O} |\Psi_{GGE}\rangle. \]

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
(\( |\Psi_{GGE}\rangle \) is parametrized in terms of the set of positive
functions \( \{ \rho_{n,k} \} \). 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
\[ \rho_{1,\lambda}(\lambda) = a_1(\lambda) + \frac{1}{2\pi} \left[ \Omega^{Q_0}(\lambda + \frac{i\eta}{2}) + \Omega^{Q_0}(\lambda - \frac{i\eta}{2}) \right]. \]

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 \( |\Psi_0\rangle \), the time-dependent expectation value of a
generic local observable \( \mathcal{O} \) can be expressed as a double
Hilbert space summation
\[ \langle \Psi(t) |\mathcal{O} |\Psi(t)\rangle = \sum_{\lambda, \lambda'} e^{-S_{\lambda} - S_{\lambda'}} e^{i(\alpha_0 - \omega_0)\tau} \langle \lambda |\mathcal{O} |\lambda'\rangle, \]
where \( S_{\lambda} = -\ln \langle \lambda |\Psi_0\rangle \). Here, \( |\lambda\rangle \) 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 thermo-
dynamic limit), one finds, in particular, that the steady-state
expectation values of observables a long time after the quench can be obtained as
\[
\lim_{t \to \infty} \lim_{\lambda \to \infty} \langle \Psi(t) | \mathcal{O} | \Psi(t) \rangle = \langle \rho_{\text{QA}}^{\psi_0} | \mathcal{O} | \rho_{\text{QA}}^{\psi_0} \rangle. \quad (12)
\]
Here $\rho_{\text{QA}}^{\psi_0}$ is an eigenstate minimizing the QA $S_{\text{QA}}[\rho] = 2S[\rho] - S_{\text{YY}}[\rho]$, where $S[\rho] = \lim_{t \to \infty} \text{Re} S_\lambda$ is the extensive real part of the overlap coefficient in the thermodynamic limit and $S_{\text{YY}}[\rho]$ is the Yang-Yang entropy of the state \cite{28,35,36}. For the Néel to XXZ quench, the exact overlaps were obtained in \cite{39} and used in \cite{21,32} to obtain the exact saddle-point densities $\rho_{\text{QA}}^{\psi_0}$ representing the steady state. Crucially, one finds \cite{21,22} that $\rho_{\text{GGE}}^{\psi_0} \neq \rho_{\text{QA}}^{\psi_0}$, 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 \cite{31} (see also \cite{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 \cite{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 \cite{31}. The starting point is the $q$-deformed $L$ operator,
\[
L(z,s) = \frac{1}{\sinh(\eta)} \left[ \sinh(z) \cosh(\eta s^z) \otimes \sigma^0 + \cosh(z) \sinh(\eta s^z) \otimes \sigma^z + \sinh(\eta)(s^- \otimes \sigma^+ + s^+ \otimes \sigma^-) \right],
\]
whose auxiliary-space components are given by $q$-deformed spin-$s$ representations with $s = 1/2, 1, \frac{3}{2}, \ldots$, obeying commutation relations $[s^+, s^-] = [2s^z]_q, [s^z, s^z] = \pm s^z$ and acting in a $(2s + 1)$-dimensional irreducible representation, $\mathcal{V}_s \simeq C^{2s+1} = \text{Isp}\{[k]; k = -s, \ldots, s\}$,
\[
s^\pm[k] = k|k\rangle, \quad s^z[k] = \sqrt{[s + 1 \pm k]_q[s \mp k]_q} |k \pm 1\rangle, \quad (14)
\]
with $[k]_q = \sinh(\eta q)/\sinh(\eta)$. By means of higher-spin auxiliary (fused) transfer matrices defined via ordered products of $L$-operators
\[
T_s(z) = \text{Tr}_s[L_{a,1}(z,s) \ldots L_{a,N}(z,s)], \quad (15)
\]
where $T_{1/2}(z) \equiv T(z)$ was used in Eq. (7) we define families of conserved operators
\[
X_s(\lambda) = r_s^{-1}(\lambda) \{ T_s(z^-) T_s(z^+) \}, \quad z^\pm = \pm \eta/2 + i\lambda. \quad (16)
\]
with $T_s(z) \equiv \partial_z T_s(z)$ and $\{ \}$ denoting the traceless part. The normalization reads $r_s(\lambda) = f[-(s + \frac{1}{2})\eta + i\lambda] \times f((s + \frac{1}{2})\eta + i\lambda)$ with $f(z) = [\sinh(z)/\sinh(\eta)]^{\Delta}$. In \cite{31} it was shown that the isotropic case that these charges are quasilocal for all $s = \frac{1}{2}, 1, \frac{3}{2}, \ldots$, and $\lambda \in \mathbb{R}$. A rigorous proof for general $\Delta > 1$ is currently under construction \cite{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 \cite{47,48,49,50} ($T$-system) for higher-spin transfer matrices,
\[
T_s(z + \frac{\eta}{2}) T_s(z - \frac{\eta}{2}) = f \left[ z + (s + \frac{1}{2})\eta \right] f \left[ z - (s + \frac{1}{2})\eta \right] + T_{s-1/2}(z) T_{s+1/2}(z), \quad (17)
\]
with the initial condition $T_{1/2}(z) \equiv f(z)$. There exists a closed-form solution to the above recurrence relation in terms of Baxter's $Q$-operators \cite{48}
\[
T_s(z) = Q \left[ z + (s + \frac{1}{2})\eta \right] Q \left[ z - (s + \frac{1}{2})\eta \right] \times \sum_{\ell = 0}^{2s} f[z + (\ell - s)\eta] \frac{Q[z + (\ell - s + \frac{1}{2})\eta]}{Q[z + (\ell - s - \frac{1}{2})\eta]}.
\]
\[
(18)
\]
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 the Bethe roots, $Q(z) = \prod_{k=1}^{\infty} \sinh(z + i\lambda_k)$. A key observation is that, in the thermodynamic limit, the spin-$s$ transfer matrix evaluated at $z^+ \ (z^-)$ is simply given by the $\ell = 0 \ (\ell = 2s)$ term in the sum in Eq. (18). This then gives
\[
\lim_{\lambda \to \infty} T_s(z^\pm) = \lim_{\lambda \to \infty} f \left[ z + (s + \frac{1}{2})\eta + i\lambda \right] \frac{Q[\mp s\eta + i\lambda]}{Q[\pm s\eta + i\lambda]}.
\]
\[
(19)
\]
The latter analysis is consistent with $\lim_{\lambda \to \infty} X_s^{-1}(\lambda) T_s(z^\pm) \times T_s(z^\pm) = 1$, representing a thermodynamic version of an inversion identity (see \cite{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
\[
\tilde{X}_s(\lambda) = T_s(\lambda) T_s(\lambda)^\dagger, \quad (20)
\]
where $T_s(\lambda)$ have the same structure as in Eq. (15) but involve $L$-operators, $L(\pm)(z, s) = L(z, s) \sinh(\eta)/[\sinh(\pm s\eta)]$. In the thermodynamic limit a quasilocal conserved operator

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\[ \hat{X}_s(\lambda) \] only differs from \( X_s(\lambda) \) by a multiple of identity, \( \hat{X}_s(\lambda) = X_s(\lambda) + t_s(\lambda) \mathbb{1} \), with \( t_s(\lambda) = [2s/(2s+1)] \times \{ \sinh (2s+1)\eta]/[\sinh^2(\eta)] \}, \lambda \). We can now define a two-parameter family of conserved charges
\[ H_s^{(n-1)}(\lambda) = \frac{1}{n!} \partial_{\lambda}^n \hat{X}_s(\lambda)|_{\lambda=0}. \]

By construction we have \([H_s^{(n)}, H_s^{(m)}] = 0\) and \([H_s^{(n)}]_{n=1}^\infty\) precisely recover the ultralocal conservation laws from Eq. (7). We thus are in a position to define the density matrix of our GGE. It is given by
\[ \hat{\rho}_{\text{GGE}} = \frac{1}{Z} \exp \left[ -\sum_{n,k=1}^\infty \beta_n^s H_s^{(n)} \right], \]

where the Lagrange multipliers \( \beta_n^s \) 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 \( \rho_{2s,2s}(\lambda) \), 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 \( \{ \hat{X}_s \}_{s=1/2}^\infty \), valid for the large system size [cf. Eq. (19)]:
\[ \hat{X}_s(\lambda) = -i \partial_\lambda \log \frac{Q(-s \eta + i \lambda)}{Q(s \eta + i \lambda)} + o(N) \]
\[ = \sum_{k=1}^M \frac{2 \sinh (2s\eta)}{\cos(2(\lambda_k + \lambda)) - \cosh(2s\eta)} + o(N). \]

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])
\[ \rho_{2s,2s}(\lambda) = a_{2s}(\lambda) + \frac{1}{2\pi} \left[ \Omega_{\psi_0}^s(\lambda + i\eta/2) + \Omega_{\psi_0}^s(\lambda - i\eta/2) \right]. \]

where \( s = \frac{1}{2}, 1, \ldots \). The right-hand side of Eq. (24) is determined by the expectation values of the quasilocal charges on the initial state,
\[ \Omega_{\psi_0}^s(\lambda) = \lim_{N \to \infty} \frac{\langle \psi_0 | \hat{X}_s(\lambda) | \psi_0 \rangle}{N}. \]

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 \( \{ \hat{X}_s \}_{s=1/2}^\infty \) completely determines the postquench stationary state through the GGE and gives the latter’s predictions identical to those coming from the QA.

**Néel quench.**—An explicit example of our construction is provided by the quench from the Néel state
\[ | \psi_0 \rangle = \frac{1}{\sqrt{2}} (| \uparrow \downarrow \uparrow \downarrow \cdots \rangle + | \downarrow \uparrow \downarrow \uparrow \cdots \rangle). \]

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.

**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 truncated 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.

**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 quasi-local charges have a non-negligible impact on the relaxation processes of strongly interacting many-body quantum systems in one dimension.

We warmly acknowledge discussions with M. Brockmann and thank him for a careful reading of the manuscript. B. W., J. D. N., and J. S. C. acknowledge support from the Foundation for Fundamental Research on Matter (FOM) and the Netherlands Organisation for Scientific Research (NWO). F. H. L. E. is supported by the EPSRC under Grants No. EP/J014885/1 and No. EP/I032487/1. This work forms part of the activities of the Delta Institute for Theoretical Physics (D-ITP). T. P. acknowledges support by Grants No. P1-0044, No. N1-0025, and No. J1-5439 of the Slovenian Research Agency.