

On Generalized Gibbs Ensembles with an infinite set of conserved charges

B. Pozsgay^{1,2}, E. Vernier³, M. A. Werner⁴

¹ Department of Theoretical Physics, Budapest University of Technology and Sciences,
1111 Budapest, Budafoki út 8, Hungary

² MTA-BME “Momentum” Statistical Field Theory Research Group,
1111 Budapest, Budafoki út 8, Hungary

³ SISSA and INFN, via Bonomea 265, 34136 Trieste, Italy

⁴ MTA-BME “Momentum” Exotic Quantum Phases Research Group,
1111 Budapest, Budafoki út 8, Hungary

August 12, 2021

Abstract

We revisit the question of whether and how the steady states arising after non-equilibrium time evolution in integrable models (and in particular in the XXZ spin chain) can be described by the so-called Generalized Gibbs Ensemble (GGE). It is known that the micro-canonical ensemble built on a complete set of charges correctly describes the long-time limit of local observables, and recently a canonical ensemble was built by Ilievski et. al. using particle occupation number operators. Here we provide an alternative construction by considering truncated GGE’s (tGGE’s) that only include a finite number of well localized conserved operators. It is shown that the tGGE’s can approximate the steady states with arbitrary precision, i.e. all physical observables are exactly reproduced in the infinite truncation limit. In addition, we show that a complete canonical ensemble can in fact be built in terms of a new (discrete) set of charges built as linear combinations of the standard ones.

Our general arguments are applied to concrete quench situations in the XXZ chain, where the initial states are simple two-site or four-site product states. Depending on the quench we find that numerical results for the local correlators can be obtained with remarkable precision using truncated GGE’s with only 10-100 charges.

1 Introduction

The equilibration of closed quantum systems has received a lot of interest recently. One of the main questions is whether the principles of statistical physics can be derived from the unitary time evolution of quantum mechanics. Can a big quantum system act as its own thermal bath, and can the emerging steady states be described by statistical physical ensembles? These problems go back to the work of von Neumann, however, our understanding of thermalization has grown considerably over the last two decades [1, 2].

An area which has received special interest is the field of integrable models. These systems possess additional conserved charges on top of the common conserved quantities. As a result the real-time dynamics of these models is more restricted and the systems can not equilibrate to standard statistical physical ensembles. In this respect they are important exceptions that deserve study on their own. However, their study is also motivated by their experimental

relevance, because they can be tailored in modern experiments [1, 3–5] and they also describe real world materials [6].

It has been proposed in [7] that integrable models equilibrate to Generalized Gibbs Ensembles (GGE’s) which involve all higher conserved charges of the systems [8–10]. The investigation of the GGE has been a central topic in this field in the last 10 years. Regarding certain non-interacting theories it was established rigorously that they indeed describe the post-quench steady states (see [11, 12] and references therein), and signs of the GGE in an almost-free model have been also observed experimentally [13].

On the other hand, less is known about genuinely interacting theories. The reason for this is that it is notoriously difficult to compute exact results for the real time evolution in these models, and typical approximation methods fail to describe the long time dynamics needed to study equilibration. Whereas it is generally believed that the GGE gives a correct description of post-quench steady states, there are a number of open questions regarding interacting theories. What is the full set of conserved charges that is required for the GGE? In practice how can one calculate predictions of the GGE? These questions have been considered on a case by case basis, and at present no general treatment is available.

An interacting model that has been investigated thoroughly is the Heisenberg XXZ model. Its importance lies in the fact that it is interacting with a tunable coupling, yet it has a relatively simple solution, and a large literature is already available to the computation of its correlation functions. Regarding the GGE the first exact results appeared in [14, 15] which gave predictions for post-quench correlators using a GGE built on the so-called ultra-local charges; a closely related work appeared later [16]. Despite the general expectation at that time that this “ultra-local GGE” should be valid, it was shown in the parallel works [17, 18] that this is not true. These works used the so-called Quench Action method [19] which is built on the knowledge of the exact overlaps with the initial states [20–23]. It was demonstrated in [17, 18] that the steady states formed in the quenches of the XXZ chain can be markedly different from the prediction of the ultra-local GGE. A complete understanding of this mismatch was finally given in [24]. It was shown there that an ensemble which also includes the recently discovered quasi-local charges [25] does in fact correctly describe the asymptotic states.

Thus, the general statements of [24] seemed to settle the status of the GGE in the XXZ chain. However, a surprising and important additional information was pointed out recently in [26]: it was shown that the canonical ensemble built out of the aforementioned local and quasi-local charges is generally ill-defined, because the Lagrange-multipliers associated to the higher charges necessarily miss certain information about the asymptotic states. This is not in contradiction with the results of [24], because the construction of [24], which correctly describes the steady states, can still be understood as a micro-canonical ensemble. As a solution to this problem, a canonical ensemble was constructed in [26] in terms of the mode occupation operators for the physical particles, whose eigenvalues are the Bethe root densities. These operators are closely related to the traditional set of conserved charges, in particular they are defined through the same set of commuting transfer matrices. While such a formulation indeed contains all necessary information about the steady-states, the role of locality in the GGE is less transparent. The mode occupation number operators have to be defined using an infinitesimal regulator, which also guarantees their quasi-locality. The physical predictions of the GGE are insensitive to this regulator, but the operators themselves that enter the GGE lose quasi-locality as the regulator is taken to zero. This is in accordance with free theories, where a GGE can be constructed using the occupation number operators, which are given by the necessarily non-local Fourier integrals.

In this work we investigate the GGE from a different point of view: we consider truncated GGE’s with only a finite number of charges. This idea goes back to the work [27] where truncated and “defective” GGE’s were considered in the Ising chain. Moreover, the paper [14] by one of the authors also considered truncated GGE’s for the XXZ chain (at that time only the ultra-local charges were included). The main goal of this work is to show that a sequence of truncated GGE’s (using both the ultra-local and quasi-local charges) can approximate

the post quench steady states with arbitrary precision. Going further, we will construct new sets of local and quasi-local charges from linear combinations of the standard ones, from which a complete GGE can be defined. It is an important aspect of this formulation that the Lagrange multipliers associated to the new charges are well defined physical state functions (“generalized temperatures”) of the spin chain. We will argue that in the infinite truncation limit all local observables are reproduced exactly, therefore our construction accomplishes the same goal as [26], although with a different set of charges. In the infinite-truncation limit the range of our operators is increased gradually and quasilocality is necessarily lost. Therefore, this limit can be understood as the counterpart of the zero-regulator limit in [26].

The article is organized as follows. In Section 2 we discuss the general principles of equilibration in quantum systems and the different statistical ensembles that can describe the long time behavior in non-integrable and integrable systems. In Section 3 we discuss the particular example of the XXZ spin chain: after a brief introduction to the solution of the model and the description of the conserved operators we present the arguments of [24], which prove that the micro-canonical ensemble correctly describe the post quench states. In section 4 we present our construction of the truncated GGE’s and prove that they can describe the steady states with arbitrary precision. Section 5 deals with concrete examples: as initial states we consider the dimer state and two different four-site product states. We present numerical evidence for the convergence of the truncated GGE’s to the micro-canonical ensemble. In the case of the four-site states we also present numerical data for the real-time evolution of local observables as obtained using the so-called iTEBD method, and a comparison is made to the predictions of the GGE.

2 Statistical ensembles for post-quench steady states

The general question underlying our work is the possibility to describe the long time behavior of local observables in an isolated quantum system following a quantum quench. For a given initial state $|\Psi_0\rangle$, the time evolution of a local observable \mathcal{O} is given by

$$\langle \mathcal{O}(t) \rangle = \langle \Psi_0 | e^{iHt} \mathcal{O} e^{-iHt} | \Psi_0 \rangle,$$

and we define the long time limit as

$$\bar{\mathcal{O}} = \lim_{T \rightarrow \infty} \int_0^T dt \langle \mathcal{O}(t) \rangle.$$

Here the averaging is introduced so that the limit is well defined even in a finite volume. If one deals with a global quench in an infinite system, then typically the averaging can be omitted.

Expanding over a set of eigenstates of the Hamiltonian H and neglecting degeneracies yields the so-called Diagonal Ensemble (DE) description,

$$\bar{\mathcal{O}} = \sum_n |c_n|^2 \langle n | \mathcal{O} | n \rangle, \quad c_n = \langle \Psi_0 | n \rangle. \quad (2.1)$$

whose accuracy has been checked for both integrable and non-integrable models [28–31]. A natural question to address is therefore that of the relation between this description and the usual ensembles of statistical mechanics.

2.1 Thermalization, micro-canonical and canonical ensembles

In equilibrium statistical mechanics, the micro-canonical ensemble average at energy E_0 of an observable \mathcal{O} is defined as

$$\langle \mathcal{O} \rangle_{\text{micro}} = \sum_n^I \langle n | \mathcal{O} | n \rangle,$$

where the restricted sum runs over eigenstates whose energies E_n are such that $|E_n - E_0| < \delta$, where the energy window δ must be small, but still much greater than the mean many-body level spacing. As discussed in [32], its precise value has no noticeable influence on the resulting value of $\langle \mathcal{O} \rangle_{\text{micro}}$. On the other hand, the Gibbs ensemble average at inverse temperature $\beta = 1/T$ is given by

$$\langle \mathcal{O} \rangle_{\text{GE}} = \frac{1}{Z} \sum_n e^{-\beta E_n} \langle n | \mathcal{O} | n \rangle, \quad Z = \sum_n e^{-\beta E_n}.$$

It is a general prediction of equilibrium statistical mechanics that in the thermodynamic limit the micro-canonical and canonical ensembles become equivalent.

In the non-equilibrium context a system is said to thermalize following a quantum quench if for all local observables

$$\bar{\mathcal{O}} = \langle \mathcal{O} \rangle_{\text{micro}} = \langle \mathcal{O} \rangle_{\text{GE}}, \quad (2.2)$$

where the above relation has to be understood in the thermodynamic limit, and where the micro-canonical average energy E_0 and canonical inverse temperature β are uniquely fixed by the conservation of energy:

$$E_0 = \langle H \rangle_{\text{GE}} = \bar{H} = \langle \Psi_0 | H | \Psi_0 \rangle. \quad (2.3)$$

In establishing (2.3) we used the fact that the Hamiltonian is itself a sum of local observables. Physically, relation (2.3) means that the temperature in the post-quench steady state is determined by the energy available in the initial state.

In generic systems, namely in the absence of further conserved quantities, a widely accepted scenario for explaining thermalization is that of the Eigenstate Thermalization Hypothesis (ETH) [30, 31], according to which the diagonal matrix elements of local operators in the eigenstates basis vary smoothly with the energy, and the off-diagonal matrix elements are exponentially small in the volume. This hypothesis can be used to prove the first equality in (2.2) as follows.

If the initial state of the quench problem satisfies the cluster decomposition principle [33] (that is, $\lim_{|x-y| \rightarrow \infty} \langle \Psi_0 | \mathcal{O}(x) \mathcal{O}(y) | \Psi_0 \rangle = \langle \Psi_0 | \mathcal{O}(x) | \Psi_0 \rangle \langle \Psi_0 | \mathcal{O}(y) | \Psi_0 \rangle$), then the variation of the energy density becomes suppressed as $\mathcal{O}(1/\sqrt{L})$:

$$\Delta \left(\frac{E}{L} \right) = \frac{1}{L} \sqrt{\langle \Psi_0 | H^2 | \Psi_0 \rangle - (\langle \Psi_0 | H | \Psi_0 \rangle)^2} \sim \frac{1}{\sqrt{L}}. \quad (2.4)$$

This means that the eigenstates having a non-negligible overlap with $|\Psi_0\rangle$ will have an energy density very close to the mean value. Together with the ETH this implies that the Diagonal Ensemble (2.1) and the micro-canonical ensemble yield the same expectation values.

The second equality in (2.2), namely the equivalence with the Gibbs ensemble, follows from analogous considerations as those of equilibrium statistical mechanics, namely the fact that in the thermodynamic limit the energy density fluctuations of the Gibbs Ensemble become negligible.

2.2 The case of integrable systems: generalized micro-canonical and generalized Gibbs ensembles

In integrable models the situation is different due to the existence of higher conserved charges $\{Q_j\}_{j=1, \dots, N_Q}$. Here N_Q denotes the number of linearly independent local charges, which typically scales polynomially with the volume of the system and therefore also goes to infinity in the thermodynamic limit.

For such models the conservation of the extra charges constrains the post-quench dynamics, therefore equilibration to the standard Gibbs ensembles cannot be expected. Instead, the so-called Generalized Gibbs Ensemble (GGE) has been put forward in [7]. In the canonical

form the GGE includes all charges with appropriate Lagrange multipliers, and the ensemble averages are defined as

$$\langle \mathcal{O} \rangle_{\text{GGE}} = \frac{1}{Z} \sum_n e^{-\sum_{j=1, \dots, N_Q} \langle n|Q_j|n \rangle \beta_j} \langle n|\mathcal{O}|n \rangle, \quad Z = \sum_n e^{-\sum_{j=1, \dots, N_Q} \beta_j \langle n|Q_j|n \rangle},$$

Following [32], a generalized micro-canonical ensemble is defined as

$$\langle \mathcal{O} \rangle_{\text{Gmicro}} = \sum_n' \langle n|\mathcal{O}|n \rangle,$$

where the restricted sum runs over all eigenstates whose charges are close to their initial expectation values,

$$|\langle n|Q_j|n \rangle - \langle \Psi_0|Q_j|\Psi_0 \rangle| < \delta_{Q_j}.$$

These generalized ensembles give a full description of the post-quench steady-state if for all local observables

$$\bar{\mathcal{O}} = \langle \mathcal{O} \rangle_{\text{Gmicro}} = \langle \mathcal{O} \rangle_{\text{GGE}}. \quad (2.5)$$

Regarding the canonical ensemble these relations can be used to fix the Lagrange multipliers through the relations

$$\langle \Psi_0|Q_j|\Psi_0 \rangle = \langle \mathcal{O} \rangle_{\text{GGE}}. \quad (2.6)$$

As for the case of thermalization discussed in the previous section, the equality (2.5) has to be understood in the thermodynamic limit. The first part of the equality, namely the equivalence between the long-time limit of local observables and the generalized micro-canonical average, can be justified similarly as in the thermal case using the so-called Generalized Eigenstate Hypothesis (GETH) [10]. The latter, whose validity has been verified in the case of the XXZ spin chain in [24], roughly states that the diagonal matrix elements of local operators depend only on the expectation values of the local charges Q_j , in other words, that if for two states all $\langle n|Q_j|n \rangle$ are close, the mean values $\langle n|\mathcal{O}|n \rangle$ will be close too. Following the same steps as in the previous paragraph, one may indeed deduce from there the equivalence $\bar{\mathcal{O}} = \langle \mathcal{O} \rangle_{\text{Gmicro}}$, given that the initial state satisfies the cluster decomposition principle.

Turning to the Generalized Gibbs Ensemble, a number of issues arise. First, we stress that in order to define the GGE one has to start from a finite volume with a finite number of charges, which means in practice that the equality (2.5) holds in the limit where both the volume of the system and the number of charges are taken to infinity. We stress that the GGE has strong predictive power even though it has an infinite set of Lagrange multipliers in the $L \rightarrow \infty$ limit: in finite volume the total number of independent parameters scales only polynomially with the volume, whereas the full Hilbert space grows exponentially.

An important concept is the so-called truncated GGE (tGGE) [14, 27]. In building the tGGE we keep a finite number of charges while taking the thermodynamic limit. The number of charges can be taken to infinity as a second step, and doing this a number of interesting physical questions can be addressed. What are the most relevant charges, which need to be added first to the tGGE? Is it possible to leave out certain charges, can these “defective” tGGE’s describe the steady states nevertheless? These questions have been investigated in the free case [14, 27], and it was found that the local observables are most influenced by the most local charges, and that the “defective” tGGE’s always miss some information about the steady states. In the XXZ chain the tGGE was first investigated in [14], however, at that time only the ultra-local charges were added to the ensemble. To our best knowledge, tGGE’s with a complete set of charges have not yet been investigated in interacting theories.

To conclude this section we put forward that in the presence of an infinite number of charges the equivalence of the micro-canonical and canonical ensembles is not guaranteed. Also, it is not clear whether the infinite number of Lagrange multipliers are physical state functions in integrable models. In a generic system with a finite number of charges the β_j have fixed physical values, such as the value of the temperature, or a chemical potential.

However, perhaps surprisingly, this is not necessarily true in an interacting system with an infinite number of charges. In the following sections we will show that the problems can be traced to inherent differences between finite and infinite dimensional configuration spaces. The questions will be discussed on the example of the spin chain.

3 The generalized microcanonical ensemble in the XXZ chain

In this section we briefly review the solution of the XXZ spin chain, the construction of its conserved charges, the GETH and the generalized microcanonical ensemble in this model. The reader who is already familiar with the technical details might skip this section.

The Hamiltonian of the XXZ Heisenberg spin chain is given by

$$H_{XXZ} = \sum_{j=1}^L (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta (\sigma_j^z \sigma_{j+1}^z - 1)) , \quad (3.1)$$

where the $\sigma_j^{x,y,z}$ are Pauli matrices acting locally on the j^{th} spin, and where periodic boundary conditions are assumed. The additive constant is chosen such that the ferromagnetic reference state $|0\rangle \equiv |\uparrow\uparrow \dots \uparrow\rangle$ is an eigenstate of H with zero energy. The number Δ is the so-called anisotropy parameter and we will use the parametrization $\Delta = \cosh(\eta)$. In the present work we will deal with the so-called massive regime where $\Delta > 1$. This limitation is chosen because of certain mathematical simplifications that arise in this regime; the details will be given below. However, we believe that the our main statements are valid for arbitrary Δ . We note that recently important progress has been made concerning the GGE in the massless regime with $|\Delta| < 1$ [34, 35].

The eigenstates of the Heisenberg model can be constructed using the different forms of the Bethe Ansatz [36, 37]. In coordinate Bethe Ansatz the wave functions can be parametrized by a set of complex quasi-momenta $\{\lambda_j\}_{j=1,\dots,N}$ (the so-called Bethe roots) as

$$|\{\lambda_j\}_{j=1,\dots,N}\rangle = \sum_{y_1 < y_2 < \dots < y_N} \phi_N(\{\lambda_j\}_{j=1,\dots,N} | y_1, \dots, y_N) \sigma_{y_1}^- \dots \sigma_{y_N}^- |0\rangle, \quad (3.2)$$

where $|0\rangle$ is the reference state with all spins up introduced above, and

$$\phi_N(\{\lambda_j\}_{j=1,\dots,N} | \{y\}) = \sum_{P \in S_N} \left[\prod_{1 \leq m < n \leq N} \frac{\sin(\lambda_{P_m} - \lambda_{P_n} + i\eta)}{\sin(\lambda_{P_m} - \lambda_{P_n})} \right] \left[\prod_{l=1}^N \left(\frac{\sin(\lambda_{P_l} + i\eta/2)}{\sin(\lambda_{P_l} - i\eta/2)} \right)^{y_l} \right]. \quad (3.3)$$

The quasi-momenta $\{\lambda_j\}_{j=1,\dots,N}$ satisfy the so-called Bethe equations, which follow from the periodicity of the wave function:

$$\left(\frac{\sin(\lambda_j - i\eta/2)}{\sin(\lambda_j + i\eta/2)} \right)^L \prod_{k \neq j} \frac{\sin(\lambda_j - \lambda_k + i\eta)}{\sin(\lambda_j - \lambda_k - i\eta)} = 1. \quad (3.4)$$

The associated energy eigenvalues are given by

$$E = - \sum_j \frac{2 \sinh^2 \eta}{\sin(\lambda_j + i\eta/2) \sin(\lambda_j - i\eta/2)}. \quad (3.5)$$

In the regime $\Delta > 1$ the solutions of the Bethe equations (3.4) are either real or assemble into regular patterns in the complex plane, the so-called strings [37]. A k -string is a set of rapidities $\{\lambda_j\}_{j=1\dots k}$ centered on the real axis and such that $\lambda_{j+1} - \lambda_j = i\eta + \delta_j$, where the deviations δ_j are exponentially small in the volume L . It can be seen from the explicit wave function (3.3) that the k -strings describe bound states of k interacting spin waves.

In the thermodynamic limit, the centers (real parts) of each type of strings become dense on the interval $[-\pi/2, \pi/2]$, and their distribution can be described by a set of continuous densities $\rho_k(\lambda)$, together with a set of densities for the corresponding holes $\rho_{h,k}(\lambda)$. The latter generalize to the interacting case the notion of hole excitations in a Fermi sea of non-interacting particles. It follows from the Bethe equations that these densities satisfy [37]

$$\rho_k + \rho_{h,k} = \delta_{k,1}s + d \star (\rho_{h,k-1} + \rho_{h,k+1}), \quad (3.6)$$

where

$$d(\lambda) = 1 + 2 \sum_{n=1}^{\infty} \frac{\cos(2n\lambda)}{\cosh(\eta n)} \quad (3.7)$$

and the convolution of two functions is defined as

$$(f \star g)(\lambda) = \int_{-\pi/2}^{\pi/2} \frac{d\omega}{2\pi} f(\lambda - \omega)g(\omega). \quad (3.8)$$

3.1 Local and quasi-local conserved charges

Conserved charges of the XXZ model can be constructed using the associated family of commuting transfer matrices. While the construction of ultra-local charges, that is, which can be written as a sum of densities with support on a finite number of lattice sites, has been known for a long time [36], it has been completed recently by the introduction a set of quasi-local charges satisfying a weaker but mathematically precise form of locality [25]. Here we just collect the main results available in the literature and refer the reader to the earlier works [24, 38–40] for more details.

The construction of the transfer matrices starts with the introduction of the so-called R-matrix, which acts on $\mathbb{C}^2 \otimes \mathbb{C}^2$ and is given explicitly as

$$R(u) = \frac{1}{\sinh(u + \eta)} \begin{pmatrix} \sinh(u + \eta) & & & \\ & \sinh(u) & \sinh(\eta) & \\ & \sinh(\eta) & \sinh(u) & \\ & & & \sinh(u + \eta) \end{pmatrix}. \quad (3.9)$$

Here u is the spectral parameter.

The fundamental monodromy matrix is constructed as

$$\tau(u) = L_M(u) \dots L_1(u),$$

where $L_j(u)$ are local Lax-operators given by

$$L_j(u) = R_{0j}(u),$$

and the index 0 stands for an auxiliary spin space. The transfer matrix is given by the trace over the auxiliary space of the fundamental monodromy matrix, namely

$$T(u) = \text{Tr}_0 \tau(u). \quad (3.10)$$

It is useful to introduce the higher spin monodromy matrices as

$$\tau_s(u) = L_M^s(u) \dots L_1^s(u),$$

where $L_j^s(u)$ are the so-called fused Lax-matrices that act on the tensor product of the physical spin at site j and an $s + 1$ dimensional auxiliary space (here and in the following we stress that s stands for twice the value of the auxiliary spin). Explicitly, $L_j^s(u)$ can be written as a 2×2 matrix acting on the j -th physical spin, such that its entries are expressed in terms of the spin- $s/2$ generators S_z^s, S_+^s, S_-^s acting on the auxiliary space [24, 39], namely

$$L_j^s(u) = \frac{1}{\sinh(u + (s+1)\frac{\eta}{2})} \begin{pmatrix} \sinh(u + \eta/2 + \eta S_z^s) & S_-^s \\ S_+^s & \sinh(u + \eta/2 - \eta S_z^s) \end{pmatrix}. \quad (3.11)$$

Higher spin transfer matrices are then defined as the trace over the auxiliary space of the monodromy matrices,

$$T_s(u) = \text{Tr}_0 \tau_s(u) .$$

In these notations $s = 1$ corresponds to the fundamental transfer matrix (3.10).

It can be proven using the famous Yang-Baxter equation [41, 42] that the transfer matrices commute for all auxiliary spin and all rapidity parameters:

$$[T_s(u), T_t(v)] = 0 .$$

This property can be used to define the conserved charges of the model. However, the discussion of the charges depends on the spin of the auxiliary transfer matrix.

The fundamental transfer matrix (3.10) gives rise to the so-called ultra-local charges of the model, which can be defined as follows. First of all it is easy to see that

$$T(0) = U ,$$

with U being the translation operator on the chain and it can be considered as the first conserved charge: $U = e^{iQ_1}$, where Q_1 is the momentum operator. The other charges can be defined as logarithmic derivatives of the transfer matrix at $u = 0$:

$$Q_j = i (\partial_\lambda)^{j-1} \log T(-i\lambda)|_{\lambda=0} . \quad (3.12)$$

It was shown in [43] that the Q_j defined this way are local in the sense that they are given as sums of products of spin variables such that they only span a finite segment of the chain of length j . We note that using the normalizations above the second conserved charge is

$$Q_2 = \frac{1}{2 \sinh \eta} H_{X X Z} . \quad (3.13)$$

The higher spin transfer matrices $T_s(u)$ can be used to define an additional set of charges through

$$X_s(\lambda) = \frac{1}{i} \partial_\lambda \log T_s(-i\lambda) , \quad (3.14)$$

where

$$Q_{s,j} = - (\partial_\lambda)^{j-1} X_s(\lambda)|_{\lambda=0} . \quad (3.15)$$

In order to have unified notation we identify $Q_{1,j} = Q_j$ with Q_j defined in (3.12). It follows from the commutativity of the transfer matrices and the identification (3.13) that all $Q_{s,j}$ are conserved under the time evolution generated by $H_{X X Z}$.

It is important that neither the rapidity-dependent $X_s(\lambda)$, nor the operators in the discrete set $Q_{s,j}$ are local in the usual sense, namely they involve contributions of arbitrarily large support on the spin chain. However, it can be shown that for all λ within the physical strip $|\Im(\lambda)| < \eta/2$, the $X_s(\lambda)$ satisfy a weaker form of locality referred to as quasi-locality [38], a mathematical definition of which can be found for instance in [25]. It is then straightforward to observe that the charges $Q_{s,j}$ defined in (3.15) are themselves quasi-local.

Most importantly, they are extensive.

The eigenvalues of the charges on Bethe states can be derived simply from the transfer matrix eigenvalues. However, strikingly simple relations have been found in [24] in the thermodynamic limit. First, for a given Bethe state let us define the generating functions

$$G_s(\lambda) = -\frac{1}{L} \langle X_s(\lambda) \rangle = \frac{1}{L} \sum_{j=1}^{\infty} \frac{\lambda^{j-1}}{(j-1)!} \langle Q_{s,j} \rangle , \quad (3.16)$$

where $\langle \cdot \rangle$ denotes eigenvalues on the corresponding Bethe state. It has been proven in [24] that for each spin s the generating function is related to the hole densities of the s -strings through

$$d \star (-a_s + \rho_{h,s}) = G_s , \quad (3.17)$$

Here a_s is a simple function given by

$$a_s(\lambda) = \frac{\sinh(s\eta)}{\sin(\lambda + is\eta/2) \sin(\lambda - is\eta/2)} = \frac{2 \sinh(s\eta)}{\cosh(s\eta) - \cos(2\lambda)}. \quad (3.18)$$

The relation (3.17) has been termed "string-charge duality" in [34], because it connects the string index to the spin of the quasi-local charges ¹.

3.2 The generalized microcanonical ensemble

The convolution in (3.17) can be inverted explicitly. If there are no poles of G_s in the physical strip then we have

$$-a_s(\lambda) + \rho_{h,s}(\lambda) = G_s(\lambda + i\eta/2) + G_s(\lambda - i\eta/2). \quad (3.19)$$

Using (3.6) we obtain

$$\rho_s(\lambda) = -G_s(\lambda + i\eta/2) - G_s(\lambda - i\eta/2) + G_{s+1}(\lambda) + G_{s-1}(\lambda). \quad (3.20)$$

The relations (3.19)-(3.20) imply that the expectation values of the conserved charges completely determine the Bethe states. In fact, it was shown in [24] that these relations can be used to prove that the generalized microcanonical ensemble gives a correct description of the steady states after quantum quenches. For the sake of completeness we reproduce this argument.

If the initial state $|\Psi_0\rangle$ is such that the variance of the conserved charges behaves as

$$\langle \Psi_0 | Q_{s,j}^2 | \Psi_0 \rangle - \langle \Psi_0 | Q_{s,j} | \Psi_0 \rangle^2 \sim \mathcal{O}(L), \quad (3.21)$$

then conservation of all $Q_{s,j}$ implies that only those Bethe states can have a non-negligible overlap with $|\Psi_0\rangle$ whose hole and root densities are calculated from (3.19)-(3.20) with

$$G_s(\lambda) = -\frac{1}{L} \langle \Psi_0 | X_s(\lambda) | \Psi_0 \rangle.$$

Relation (3.21) is guaranteed for states satisfying the cluster decomposition principle. On the other hand, it has been known since the early research on Algebraic Bethe Ansatz that the root and hole densities completely determine the expectation values of local observables [36]. Also, an explicit and efficient way to compute so-called factorized formulas for the correlators has been presented in [45].

It follows from the above that the first assumption of the Generalized Eigenstate Thermalization Hypothesis is valid in the XXZ spin chain: the expectation values of local observables only depend on the macroscopic values of the complete set of conserved charges. The second assumption concerning the sufficiently fast decay of the off-diagonal matrix elements has to be investigated separately, and there are cases when it is indeed not satisfied ². However, in those cases when the second assumption also holds the GETH implies immediately that the microcanonical GGE using the full set of conserved charges is indeed correct.

It is interesting to note that the overall magnetization is completely determined by the set of charges, which follows directly from (3.20). Therefore the conserved operator S^z is not independent in this approach.

¹We note that the idea that the spin of a fused transfer matrix can correspond to a string index already appeared earlier in the literature, for example in [44] where the equivalence of the so-called Quantum Transfer Matrix and Thermodynamic Bethe Ansatz methods was studied.

²Although not treated in this paper, the off-diagonal matrix elements are responsible for the lack of symmetry restoration in certain cases when the initial state does not share the symmetries of the Hamiltonian.

4 Building the canonical GGE in the XXZ chain

In this section we move to the core of the present work, which is to investigate whether the steady-states produced by quantum quenches can be described using a (canonical) Generalized Gibbs Ensemble. In the previous section we have already seen that the generalized microcanonical formulation is correct, since the expectation values of local and quasi-local conserved charges in the initial state $|\Psi_0\rangle$ completely determine all root densities $\rho_k(\lambda)$, which are the only physical information needed to describe the local observables in the thermodynamic limit. Therefore, the remaining question is whether there is a canonical ensemble which produces Bethe states with the desired root densities $\rho_k(\lambda)$.

4.1 The canonical GGE

We start with the most natural construction of a canonical GGE in terms of the local and quasi-local charges $Q_{s,j}$ introduced in the previous section. For the purpose of all computations it is in fact necessary to start from a finite number of charges, therefore we define a sequence of truncated GGE (tGGE) density matrices as

$$\varrho_n = \frac{1}{Z} \exp \left(- \sum_{s=1}^{N_s(n)} \sum_{j=1}^{N_d(n)} \beta_{s,j} Q_{s,j} \right), \quad (4.1)$$

where the parameters $N_s(n)$ and $N_d(n)$ are truncation numbers, which depend on the sequence index n , and Z always denotes the partition function such that $\text{Tr} \varrho_n = 1$. The parameters $N_s(n)$ and $N_d(n)$ could in principle depend on the volume, however, in the present work we follow the approach that the thermodynamic limit is performed first with fixed truncation numbers. In order to capture all information of the steady states eventually one has to add an infinite number of charges, therefore the correct density matrix should be reached in the $n \rightarrow \infty$ limit, where both $N_{s,d}(n) \rightarrow \infty$, even though the specific way of approaching infinity is not specified at this stage.

The truncated GGE with only the ultra-local charges ($N_s = 1$) was first studied in [14]. In that case the choice for increasing N_d gradually is physically motivated: higher charges are less and less local, and it was already expected in [27] that they would have decreasing influence on short-range observables. In fact, this was observed in [14], even though a general theoretical proof for this behaviour is still missing. For the quasi-local charges it is not immediately evident why one should add the charges with small derivative indices first, since for a given value of the auxiliary spin $s > 1$ all these charges are sums of densities with arbitrarily large range. More precisely one can write

$$Q_{s,j} = \sum_i \mathcal{P}_i \left(\sum_{r \geq 2} q_{s,j}^{[r]} \right), \quad (4.2)$$

where the first sum runs over the lattice sites and the operator $\mathcal{P}_i(\dots)$ denotes a translation by i lattice sites, while the densities $q_{s,j}^{[r]}$ have a non-trivial action on r consecutive lattice sites only and act as identity on the rest of the chain. For a given $s > 1$ the norm of these densities is known [25] to decay exponentially with r , with a rate independent of the derivative index j . Despite this fact, we can argue that, as the ultra-local charges corresponding to $s = 1$, the quasi-local charges become “less and less local” when j is increased. This can be seen, for instance, by looking at the average ranges $\bar{r}_{s,j}$ of these charges, which we define as (see also [46])

$$\bar{r}_{s,j} = \frac{\sum_{r \geq 2} r \|q_{s,j}^{[r]}\|_{\text{HS}}^2}{\sum_{r \geq 2} \|q_{s,j}^{[r]}\|_{\text{HS}}^2}, \quad (4.3)$$

where $\|\cdot\|_{\text{HS}}$ denotes the Hilbert-Schmidt norm. On figure 1, we report the values of $\bar{r}_{s,j}$ for $s = 1$ and $s = 2$, as a function of the derivative index j . Both in the ultra-local ($s = 1$) and

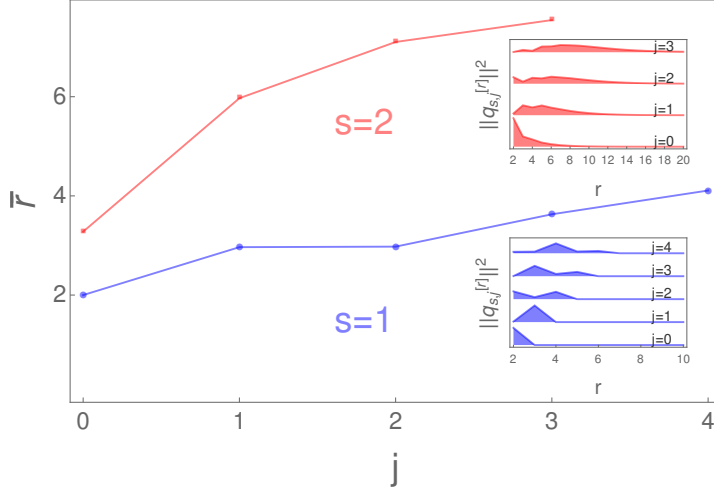


Figure 1: Average range (4.3) of the charges $Q_{s,j}$ for $s = 1$ and $s = 2$ respectively, plotted as a function of the derivative index j for the first few values of j . The anisotropy parameter of the model is taken to be $\eta = 1$. In inset we have represented the Hilbert-Schmidt norms $\|q_{s,j}^{[r]}\|_{\text{HS}}^2$ of the corresponding densities as a function of the range r .

quasi-local ($s = 2$) cases, these are indeed seen to increase with j . This motivates building a truncated GGE starting from the smallest values of j , and the usefulness of this approach will further become evident from our calculations presented below.

4.2 Review of the results of Ilievski *et. al.*

An alternative way towards a canonical GGE is considered in [26], where the full rapidity dependent family of quasi-local charges $\{X_s(u)\}$ is added directly to the GGE density matrix. In this case the Lagrange-multipliers also become functions of the rapidity variable u . The density matrices can be written as

$$\varrho = \frac{1}{Z} \exp \left(- \sum_{s=1}^{N_s} \int_{-\pi/2}^{\pi/2} du \lambda_s(u) X_s(u) \right). \quad (4.4)$$

These densities matrices were analyzed in [26] using the Thermodynamic Bethe Ansatz (TBA) method [37]. Introducing the standard functions $Y_s(u) = \rho_{h,s}(u)/\rho_s(u)$ which can be interpreted as the analogue of the (inverse) filling fractions of free theories, the resulting Bethe states were shown to satisfy

$$\log(Y_s) = \lambda_s \star d + d \star (\log(1 + Y_{s+1}) + \log(1 + Y_{s-1})), \quad (4.5)$$

It was shown in [26] that the solution of (4.5) satisfies to so-called modified Y -system relations

$$Y_s^+ Y_s^- = e^{\lambda_s} (1 + Y_{s-1})(1 + Y_{s+1}), \quad (4.6)$$

where we introduced the notation $f^\pm(u) = \lim_{\varepsilon \rightarrow 0} f(u \pm i(\eta/2 - \varepsilon))$. This relation is easily obtained using the pseudo-inverse of the convolution with d , which can be defined as [26]

$$(d^{-1}f)(u) = f^+(u) + f^-(u). \quad (4.7)$$

It follows from the Fourier decomposition of u that $d^{-1}d \star f = f$ for all functions and indeed this leads to (4.6) immediately. However, $d \star d^{-1}f$ is only equal to f if it does not have any poles in the physical strip.

As a consequence of (4.6), it was argued in [26] that the canonical GGE (4.4) can not describe the post-quench steady states. Probably the simplest way to see this is to consider initial states that are products of local two-site states, in which cases exact solutions for the Y -functions are known [39, 47, 48]. It has been demonstrated earlier and finally proven in [49] that they satisfy the original Y -system

$$Y_s^+ Y_s^- = (1 + Y_{s-1})(1 + Y_{s+1}). \quad (4.8)$$

It follows that if a GGE of the form (4.4) would require $\lambda_s \equiv 0$ in order to describe these states, which is an apparent contradiction.

It has been pointed out in [26] that the reason for this mismatch is that the Lagrange-multipliers $\lambda_s(u)$ necessarily miss certain information which can be encoded in the ensembles that use the root density operators directly:

$$\varrho = \frac{1}{Z} \exp \left(- \sum_{s=1}^{\infty} \int_{-\pi/2}^{\pi/2} du \, \mu_s(u) \hat{\rho}_s(u) \right), \quad (4.9)$$

where

$$\hat{\rho}_s(u) = \lim_{\varepsilon \rightarrow 0^+} [X_s(u + i\eta/2 - i\varepsilon) + X_s(u - i\eta/2 + i\varepsilon) - X_{s+1}(u) - X_{s-1}(u)]. \quad (4.10)$$

It follows from (3.17) that the eigenvalues of the operators $\hat{\rho}_s(u)$ are the Bethe root densities $\rho_s(u)$, given that the functions $X_s(u)$ don't have poles in the physical strip. Considering the density matrices (4.9) in the Bethe Ansatz basis it is evident that they can produce arbitrary post-quench states, because the Lagrange-multipliers are coupled to the root densities directly.

The infinitesimal regulator in (4.10) plays an important role: the operators $\rho_s(u)$ are well-defined and quasi-local only for $\varepsilon > 0$. On the other hand, quasi-locality is lost in the $\varepsilon \rightarrow 0$ limit. This is in accordance with free theories, where the particle number operators are Fourier modes of the free fields, which are inherently non-local quantities. The operators $\hat{\rho}_s(u)$ provide an exact resolution of the particle densities in rapidity space, which requires infinite integration in real space. On the other hand, restricting the range of the operators to a finite length L would result in smeared densities with precision $\varepsilon = 1/L$.

Coming back to the truncated GGE's introduced in the previous paragraph, it is tempting to identify the integral form $\int \lambda_s(u) X_s(u)$ with the $N_d \rightarrow \infty$ limit of the sequence (4.1). However, there are a number of subtle issues regarding this identification. Assuming that the identification can be established, it follows from the results of [26] that the tGGE of the form (4.1) can not describe the post-quench steady-states. This motivate us to relax the requirement that the Lagrange multipliers $\beta_{s,j}$ should have fixed values independent of the truncation index. In the next section we will show that if we allow for *varying* $\beta_{s,j}(n)$ as a function of the truncation index n , then this way we can describe all Bethe root distributions. On the other hand, if the $\beta_{s,j}$ are allowed to vary with n , the resulting tGGE can not be identified with (4.4) anymore.

The original construction (4.1) reflects physical intuition from standard non-integrable systems, where the finite number of Lagrange multipliers are actual state functions and have well defined physical values. In integrable models the situation is different due to the infinite number of charges. We will show that the unphysical nature of the varying $\beta_{s,j}$ can be remedied by constructing a new set of charges, so that the associated Lagrange multipliers become well defined state functions. Moreover, we expect that our construction is an alternative way towards the $\varepsilon \rightarrow 0$ limit of the GGE density matrix (4.9).

4.3 Construction of truncated GGEs

According to the discussion above we consider sequences of tGGE's where each $\beta_{s,j}$ is allowed to depend on the truncation index n , namely

$$\varrho_n = \frac{1}{Z} \exp \left(- \sum_{s=1}^{N_s(n)} \sum_{j=1}^{N_d(n)} \beta_{s,j}(n) Q_{s,j} \right). \quad (4.11)$$

There are two approaches to fixing the Lagrange multipliers. One possibility is to require that at each truncation step the operators that are already added will acquire the correct mean values dictated by the initial state:

$$\text{Tr}(\varrho_n Q_{s,j}) = \langle \Psi_0 | Q_{s,j} | \Psi_0 \rangle, \quad s = 1, \dots, N_s(n), \quad j = 1, \dots, N_d(n). \quad (4.12)$$

Regarding the ultra-local charges this approach was considered in [14]. The alternative approach is to relax (4.12) and only require that the charges obtain the correct values in the infinite truncation limit:

$$\lim_{n \rightarrow \infty} \text{Tr}(\varrho_n Q_{s,j}) = \langle \Psi_0 | Q_{s,j} | \Psi_0 \rangle, \quad s = 1, \dots, \infty \quad j = 1, \dots, \infty. \quad (4.13)$$

It follows from the string-charge duality (3.17) that this merely means that in the $n \rightarrow \infty$ limit the correct $\rho_k(u)$ Bethe root distributions are reproduced.

In the present work we will follow the second approach, because it enables us to perform certain mathematical steps more easily. However, we stress that from a physical point of view the two approaches can be considered equivalent, because eventually we will be interested in the physical quantities in the $n \rightarrow \infty$ limit, when both the local and quasi-local quantities will take their correct physical values.

Using once again a TBA strategy, the density matrices of the type (4.11) produce states satisfying

$$\log(Y_s) = -\delta_{s \leq N_s} \sum_{k=1}^{N_d} \beta_{s,k} d^{(k)} + d \star (\log(1 + Y_{s+1}) + \log(1 + Y_{s-1})), \quad (4.14)$$

where

$$d^{(k)}(u) = \left(\frac{d}{du} \right)^{k-1} d(u).$$

Note that in both TBA equations (4.5) and (4.14), the spin index of the Lagrange multipliers is identified with the string index of the Y -function, and this is analogous to the relation (3.17). Moreover, the structure of the individual source terms reflects the definition of the charges entering the GGE's.

Our claim now is that any post-quench steady-state can be described this way. More precisely, we will argue that the following proposition is true:

Proposition 1 *For any initial state $|\Psi_0\rangle$ with well defined charges there exists a sequence of tGGE's*

$$\varrho_n = \frac{1}{Z} \exp \left(- \sum_{s=1}^{N_s(n)} \sum_{j=1}^{N_d(n)} \beta_{s,j}(n) Q_{s,j} \right), \quad (4.15)$$

such that the local observables in the post quench steady state will be given by the infinite truncation limit

$$\lim_{T \rightarrow \infty} \int_0^T dt \langle \mathcal{O}(t) \rangle = \lim_{n \rightarrow \infty} \langle \varrho_n \mathcal{O} \rangle.$$

The rest of this section will be devoted to the proof of this proposition, and to analyze the corollaries of the proof.

The mean values of local correlators in the Bethe states only depend on the root densities [36, 45], therefore it is enough to prove the following:

Proposition 2 *For any Bethe root distribution $\{\rho_k(u)\}$ there exists a sequence of tGGE's*

$$\varrho_n = \frac{1}{Z} \exp \left(- \sum_{s=1}^{N_s(n)} \sum_{j=1}^{N_d(n)} \beta_{s,j}(n) Q_{s,j} \right), \quad (4.16)$$

such that, for real u ,

$$\lim_{n \rightarrow \infty} \rho_k^n(u) = \rho_k(u), \quad (4.17)$$

where $\rho_k^n(u)$ is the sequence of root densities obtained from ϱ_n . In (4.17) the convergence is understood in L_2 norm, but it is not necessarily uniform in the string index k .

The main idea of the proof of this proposition is to write down a fictitious TBA satisfied by the physical root densities and to approximate the fictitious source terms using the discrete set of charges. To this end we write down a TBA-like equation and look for the apparent sources:

$$\log \frac{\rho_{h,s}(u)}{\rho_s(u)} = \delta_s(u) + d \star \left[\log \left(1 + \frac{\rho_{h,s-1}(u)}{\rho_{s-1}(u)} \right) + \log \left(1 + \frac{\rho_{h,s+1}(u)}{\rho_{s+1}(u)} \right) \right]. \quad (4.18)$$

Here the functions $\delta_s(u)$ are merely some remainder functions determined from the physical root densities, which in turn are determined from the charges of the initial state through relation (3.17).

The idea is to construct a series of TBA equations of the form (4.14) which will approximate the source terms $\delta_s(u)$ with arbitrary precision. This can be achieved by noting that the source terms in (4.14) involve linear combinations of all the derivatives of the function $d(u)$. For such situations the following theorem holds:

Theorem 1 *Let $d(u) \in L_2([-\pi/2, \pi/2])$ such that all of its Fourier components are non-zero. Let D be the set of functions formed from $d(u)$ and its derivatives:*

$$D = \{d(u), d'(u), d''(u), \dots\}.$$

Then the linear span of D is dense in $L_2([-\pi/2, \pi/2])$. In other words, for any function $f \in L_2([-\pi/2, \pi/2])$ there is a sequence

$$f_n = \sum_{j=1}^n \alpha_j(n) d^{(j-1)}, \quad (4.19)$$

such that $\lim_{n \rightarrow \infty} f_n = f$.

The proof to this theorem was given by Christian Remling at the website Math.Stackexchange [50]. The technical details of the proof are not relevant to the content of this paper, therefore we do not reproduce the proof here. However, we stress that it is essential that all Fourier components of $d(u)$ are non-zero: any missing Fourier mode would be outside the linear span of the set D .

It is important to clarify in what sense D can or can not be considered a basis in $L_2([-\pi/2, \pi/2])$. One of the common concepts for infinite dimensional spaces is the Schauder basis, whose definition is the following. A set $\{b_j\}$ of vectors of a Banach space is a Schauder basis, if for every vector v there is a unique set of coefficients $\{\alpha_j\}$ such that

$$v = \lim_{n \rightarrow \infty} \sum_{j=1}^n \alpha_j b_j.$$

In the present case it can be shown that the set D is not a Schauder basis of $L_2([-\pi/2, \pi/2])$. In fact, the coefficients of the approximating sequence (4.19) typically vary with n . To prove that D can not be a basis it is enough to show that one of its elements can be approximated with arbitrary precision using the remaining functions. This is easily seen by considering the

set $D_2 = \{d'', d''', d''', \dots\}$, which is of the same type as D except that the constant terms of all functions are zero. It follows that any function whose integral is zero can be approximated using D_2 . We can apply this argument to d' . It follows that the expansion of a function f using the elements of D can not be unique, therefore D can not be a Schauder basis. This has interesting physical consequences, which will be discussed below.

Returning to the construction of the approximating TBA, Theorem 1 can be applied directly to the approximation of the individual source terms $\delta_s(u)$ in (4.14). This means that it is possible to obtain a sequence of sets of Lagrange-multipliers, such that for each s

$$\delta_s(u) = \lim_{n \rightarrow \infty} \left(\sum_{j=1}^n \beta_{s,j}(n) d^{(j-1)}(u) \right). \quad (4.20)$$

In the tGGE's (4.11) there are always a finite number of charges included, so it is not possible to approximate all source terms at the same time. Instead, both N_s and N_d have to be increased gradually. This can be performed in many ways, the simplest one is probably to set $N_s = N_d = n$. Doing this we only approximate the first n nodes of the TBA equations, and the remaining ones will be left with vanishing source, as in the case of the thermal TBA. One might ask whether this approximation scheme is sufficient to obtain correct values for the physical observables.

It is a general experience with the TBA that the influence of the sources for the higher strings on the root densities of the smaller strings is small. Also, the root densities of the higher strings typically don't change the values of the local correlators; in fact all local correlators can be expressed using the 1-string nodes of certain auxiliary functions only [45, 48]. It follows that a gradual increase of N_s and N_d will result in the correct values of the local correlators, even if the convergence of the sources and root densities is not uniform in the string index. At present we can not make this argument mathematically precise, therefore we also demonstrate this approximation procedure on concrete examples in the next section.

An important technical issue is the asymptotic behavior of the TBA for large string indices. It is known that depending on the situation the asymptotics can be very different [24, 37, 39, 47, 49]. However, it is expected that if all low lying TBA nodes have the correct non-trivial source terms, then a large class of asymptotic behaviors will lead to the same root densities in the infinite truncation limit.

In the remainder of this section we present a few remarks and questions regarding our construction of the tGGE's.

- It is interesting to consider the Lagrange multipliers with the lowest derivative index. To do this we integrate equation (4.20) and obtain

$$\lim_{n \rightarrow \infty} \beta_{s,1}(n) = \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} du \delta_s(u). \quad (4.21)$$

This means that all $\beta_{s,1}$ have well defined physical values determined by the post-quench steady state, and therefore they could be considered state functions. Quite interestingly this includes the parameter $\beta_{1,1}$ which is the coefficient of the Hamiltonian in the GGE, and therefore can still be identified with the inverse temperature. In our numerical investigations (to be presented in section 5) we found that all other $\beta_{s,j}$ typically oscillate and indeed only $\beta_{s,1}$ tend to fixed values. We will however see in the next subsection that linear combinations of the $\beta_{s,j}$'s can be formed, which have well defined values and can therefore be interpreted as "generalized inverse temperatures".

- It is worthwhile to consider the Y -system equations. The TBA (4.14) following from the tGGE's necessarily leads to Y -functions that satisfy the original relation (4.8); this can be proven in at least two ways. One possibility is the formal manipulation of the TBA itself, leading to an equation of the form (4.6) with the $\lambda_s(u)$ being composed of Dirac-deltas and its derivatives. These singularities appear at the isolated points

$u = 0$ and are removable. The other way to prove the Y -system is to construct the Quantum Transfer Matrix (QTM) associated to the tGGE's, and then the Y -system follows from the fusion hierarchy, in complete analogy with the simple thermal case [44]. The QTM method has been already applied to a tGGE's including the ultra-local charges in [14, 15]. The addition of the quasi-local charges leads to a QTM which acts on a spin chain with mixed higher spins. However, the Y -system relations are not modified by this, and they hold in the original form for all tGGE's³.

Quite interestingly, a generic quantum quench leads to root densities and Y -functions that do not satisfy the Y -system. In fact, the root densities and Y -functions are determined from the charges, and generally there is no reason for the Y -system to hold, unless there is some additional integrable structure associated to the particular initial state. In the case of the two-site product states this algebraic structure is the fusion hierarchy of the corresponding Boundary Quantum Transfer Matrix [49]. The atypicality of such states has been mentioned in [34], and it was first observed in [39] that for certain four-site product states the Y -system is indeed violated.

It is then a natural question to ask, how can the tGGE's approximate the physical root densities, given that they satisfy the Y -system at each truncation step. The answer is that the convergence of the approximating root densities $\rho_s^{(n)}(u)$ is typically not uniform in the rapidity parameter. The Y -system involves a shift of $\pm\eta/2$ in the imaginary direction, which does not necessarily commute with the infinite truncation limit. In fact, our tGGE's are constructed so that they approximate the root density functions on the real line, because this is the only information which is needed to obtain the correct predictions for the local observables. On the other hand, they can have a different behavior in the complex plane. This is easily seen in the examples to be considered in section 5. The true source terms for the TBA typically have log-zero and/or log-infinity singularities. It is possible to approximate such functions using our set D , but the analytic properties of the approximating functions will be markedly different. For example there is no actual singularity at any finite truncation step, and the log-singularities are not approached uniformly. Moreover, the Y -functions resulting from the tGGE's are only convergent on the real axis.

- Our construction operates in the space of the source terms for the TBA equations. However, it is natural to ask what is the closure of the linear span of the set $\{Q_{s,j}\}$ in the space of operators, and to which operators do the exponents in our sequences of tGGE's converge.

Any finite linear combination of the $Q_{s,j}$ is an operator which is conserved and quasi-local, but it needs to be investigated whether these properties are preserved by our limiting procedures. We conjecture that the commutativity with the Hamiltonian holds even for the closure of the linear span of the set $\{Q_{s,j}\}$. On the other hand, the quasi-locality property can be violated, which follows from the fact that the original rapidity dependent family $X_s(u)$ is only quasi-local inside the physical strip with $|\Im u| < \eta/2$.

As it was already remarked above, in [26] a canonical GGE was built using the particle density operators, as given by eq. (4.9). Whereas this GGE correctly captures the post-quench steady states, all the terms in the exponent lose their quasi-locality as the regulator ε is sent to zero. It is then natural to conjecture that the limit of our sequences of tGGE's actually coincides with the zero-regulator limit of (4.9). If this is indeed true, it means that our construction is another way to approximate the inevitably non-local exponent of the GGE using physically acceptable, quasi-local operators.

- It is also useful to compare our results to the original formulation of the complete GGE (4.4), which was proven to be not viable in [26]. Comparing the fictitious TBA (4.18) to (4.5) we find that the original formulation can only describe the Bethe root densities if

$$d \star \lambda_s = \delta_s. \quad (4.22)$$

³We are grateful to Junji Suzuki for discussions about these questions.

However, as explained in [26], the convolution with d does not have an inverse, therefore (4.22) can not be satisfied for an arbitrary quench problem.

Within our approach the fictitious source terms are approximated with the function d and its derivatives. At any finite truncation (4.22) can be satisfied if we allow the λ_s to become distributions instead of analytic functions. In particular, if for a given truncation index n

$$\delta_s(u) \approx \sum_{j=1}^n \beta_{s,j}(n) d^{(j-1)}(u),$$

then we have

$$\lambda_s \approx \sum_{j=1}^n \beta_{s,j}(n) \delta^{(j-1)},$$

with δ being the Dirac-delta.

As explained above, the coefficients $\beta_{s,j}(n)$ typically do not have a $n \rightarrow \infty$ limit, therefore the formulation (4.5) is ill-defined even if we allow the Lagrange-multipliers to become distributions.

- We note an interesting consequence of our construction: It is possible to leave out any finite number of charges from the tGGE's, given that the first members $Q_{s,1}$ are included for any spin index s . This is most easily seen on the example of the set $D' = D \setminus \{d'\} = \{d, d'', d''', d''', \dots\}$. It can be proven that all source terms of the TBA (4.14) can be approximated using D' only: the first member d can be used to correctly fit the constant terms of $\delta_s(u)$, and the set $D_2 = \{d'', d''', d''', \dots\}$ is sufficient to approximate the remainder. A similar argument shows that in fact any other finite number of charges can be left out, as long as the first member $Q_{s,1}$ is always included. Such GGE's with missing charges were already studied in the case of the Ising model in [27]. There it was found that leaving out certain charges does have an effect on the mean values of local correlators, which is in contradiction with our results. This contradiction can be traced to the fact that in the free theories the relevant set of source functions simply consists of Fourier modes, therefore it is a Schauder basis, which is not true in the interacting case.

We also remark that the omission of a finite number of charges has an effect on the speed of convergence of the tGGE. Leaving out one or two charges, there are more and more operators needed to reach the full microcanonical predictions with the same accuracy. This is demonstrated on the example of the dimer state in section 5.

4.4 Identification of physical state functions

In the previous paragraphs, we have seen that the sequence of truncated GGE's of the form (4.1) cannot reproduce properly the steady-state properties after a generic quantum quench, unless the Lagrange multipliers $\beta_{s,j}$ (for $j > 1$) are allowed to vary with the truncation index n . In other terms, for $j > 1$ these do not have a well-defined value in the $n \rightarrow \infty$ limit, and therefore cannot be considered as physical state functions. We will now show, as a corollary of our construction, that state functions can in fact be built.

In practice the approximation of the source terms of the TBA can be performed using an orthonormal basis of functions $\tilde{D} = \{\tilde{d}_j\}_{j=1,\dots,\infty}$ which is obtained from D by Gram-Schmidt orthogonalization procedure with respect to the usual L_2 norm :

$$\tilde{d}_j = A_{jk} d_k, \quad \text{where } A_{jk} \neq 0 \quad \text{for } j \geq k,$$

and

$$(\tilde{d}_j, \tilde{d}_k) \equiv \int_{-\pi/2}^{\pi/2} du \tilde{d}_j(u) \tilde{d}_k(u) = \delta_{jk}. \quad (4.23)$$

A numerical example for the linear transformation is given below (here $\Delta = 3$):

$$A = \begin{pmatrix} 0.50885 & & & & \\ 0.21118 & 0.25771 & & & \\ 0.10332 & 0.27570 & 0.02683 & & \dots \\ 0.05379 & 0.27368 & 0.04831 & 0.00115 & \\ 0.02903 & 0.28385 & 0.06799 & 0.00293 & 0.00003 \\ & & \vdots & & \ddots \end{pmatrix}.$$

It follows from the completeness of D and the orthogonality condition (4.23) that \tilde{D} is a Schauder basis, i.e. every source term $\delta_s(u)$ in the TBA (4.14) has a unique expansion

$$\delta_s(u) = \sum_{j=1}^{\infty} \tilde{\beta}_{s,j} \tilde{d}_j(u), \quad (4.24)$$

where the Lagrange multipliers are determined simply from

$$\tilde{\beta}_{s,k} = \int_{-\pi/2}^{\pi/2} du \tilde{d}_k(u) \delta_s(u).$$

Resultingly, the TBA equations (4.14) can be rewritten as

$$\log(Y_s) = -\delta_{s \leq N_s} \sum_{k=1}^{N_d} \tilde{\beta}_{s,k} \tilde{d}_k + d \star (\log(1 + Y_{s+1}) + \log(1 + Y_{s-1})). \quad (4.25)$$

It follows from the structure of the source terms in (4.14) that the equivalent TBA's (4.14)-(4.25) can be interpreted as generated by a sequence of truncated GGE's of the form

$$\varrho_n = \frac{1}{Z} \exp \left(- \sum_{s=1}^{N_s(n)} \sum_{j=1}^{N_d(n)} \tilde{\beta}_{s,j} \tilde{Q}_{s,j} \right), \quad (4.26)$$

where the new set of charges is defined using the same linear transformation:

$$\tilde{Q}_{s,j} = A_{jk} Q_{s,k} \quad s = 1, 2, \dots, \quad (4.27)$$

and where for each truncation index n we have the requirement

$$\sum_{j=1}^n \beta_{s,j}(n) Q_{s,j} = \sum_{j=1}^n \tilde{\beta}_{s,j} \tilde{Q}_{s,j}.$$

It follows that the $\{\tilde{\beta}_{s,j}\}$ are related to the $\{\beta_{s,j}\}$ through

$$\beta_{s,j}(n) = \sum_{k=1}^n A_{kj} \tilde{\beta}_{s,k}. \quad (4.28)$$

The new discrete set of operators $\{\tilde{Q}_{s,j}\}$ can serve as the basis of the GGE in the usual sense, namely

$$\varrho = \lim_{n \rightarrow \infty} \frac{1}{Z} \exp \left(- \sum_{s=1}^n \sum_{j=1}^n \tilde{\beta}_{s,j} \tilde{Q}_{s,j} \right), \quad (4.29)$$

where each Lagrange multiplier has a well defined value and therefore plays the role of a physical state function. For a given truncation index n the $\tilde{\beta}_{s,j}$ may be written as a linear combination of all the $\beta_{s,j'}$ with $j \leq j' \leq n$, and similarly, the $\beta_{s,j}$ may be written as a linear

combination of all the $\tilde{\beta}_{s,j'}$ with $j \leq j' \leq n$. It follows from (4.28) that even though the $\tilde{\beta}_{s,j}$ have a well defined (n -independent) value, this is not the case for the $\beta_{s,j}$, and in fact they might not converge in the $n \rightarrow \infty$ limit.

Conversely, the charges $\tilde{Q}_{s,j}$ (whose construction does not depend on the truncation index n , neither on the considered initial state) are linear combinations of the $Q_{s,j'}$ for $j' \geq j$, so they inherit from the (quasi)locality properties of the latter.

We remark that even though all quantities are well defined and finite in (4.29), the resulting density matrix is still to be understood as an infinite truncation limit. As a result, the TBA calculations have to be restricted to the real line, because analytic continuation into the complex plane typically does not commute with the infinite truncation limit.

An important aspect of the set $\{\tilde{Q}_{s,j}\}$ is that all charges are required to properly reproduce the post-quench properties. This clearly stems from the orthogonality property of the set \tilde{D} , namely removing one function from this set makes impossible to reconstruct a generic source term $\delta_s(\lambda)$. This contrasts with the case of the charges $\{Q_{s,j}\}$, for which we have argued in the previous paragraph that a defective sequence of tGGE's may in the generic (interacting) case still correctly reproduce the post-quench properties, albeit with a slower convergence.

To conclude this section, let us point out that while the construction of the set $\{\tilde{Q}_{s,j}\}$ is independent of the considered initial state, its choice is in fact not unique. Indeed, if the Gram-Schmidt orthogonalization is performed on a set D' where a finite number of elements of D are left out, we obtain a different set of modified charges. In practice this means that there are multiple ways to obtain a set of operators which serves as a ‘‘Schauder-like’’ basis for the GGE, meaning that all coefficients will have fixed finite values for all initial states once the operators are fixed. However, there remains a certain amount of ambiguity in choosing the operators themselves. As it was remarked above, the omission of certain elements of D leads to a slower convergence of the tGGE, therefore the physically motivated choice is to include all elements of D , and this selects a particular set of modified charges. Another possibility for constructing the set $\{\tilde{Q}_{s,j}\}$ is to use a different choice for the inner product in the space of source functions. All of these choices are expected to lead to different sets of physical charges $\{\tilde{Q}_{s,j}\}$, and conversely, to different sets of state functions $\{\tilde{\beta}_{s,j}\}$. However, all of these choices are linearly related, therefore equally physical.

5 Examples

Here we numerically investigate the approximation procedure introduced in the previous section using concrete examples. For the quenches we consider initial states that are products of local states spanning a few sites. The reasons for choosing such states is twofold. First, they could be tailored in experiments, partly due to their simple structure, or because they are ground states of simple local Hamiltonians. The second reason for choosing such states is that there are exact methods available to compute the conserved charges in these states [15, 24], which makes their numerical treatment relatively easy.

We aim to show that it is indeed possible to construct a sequence of tGGE's of the form (4.11) such that the local correlators will approach their steady state values as the truncation index n is increased. In section 3 it was explained that the microcanonical GGE is correct in the XXZ model, therefore in principle it is enough to demonstrate that the tGGE's produce root densities that converge to the physical $\rho_k(u)$ as obtained from the charges. However, for an easier comparison (and also due to their physical importance) we will investigate the convergence of the local correlators.

Our concrete examples are the so-called dimer state and two different four-site states; they will be investigated in subsections 5.1 and 5.2, respectively. The dimer state has already been studied extensively [18, 48, 51], but there are fewer results available for the four-site states.

As it was already pointed out in [39], in the case of four site states the resulting Y -functions (denoted as η -functions in [39]) typically do not satisfy the Y -system equations (4.8), and this motivates their detailed study. In [39] exact results were derived for the root

densities in the case of a particular four-site state (the so-called 4-site domain wall state), however, real time evolution in these cases has not yet been considered before. Our goals are twofold. First we intend to demonstrate that our construction of the truncated GGE's is independent of the Y -system relations and also works when these do not hold. Second, we aim to check the validity of the full microcanonical GGE. Therefore we also perform a simulation of the real time evolution using the iTEBD method [52–54]; the details of the method have been described in our previous works [18, 48]. Even though there is no reason to expect any deviations from the GGE predictions, we believe it is useful to present these numerical results as well.

Our methods are the following. For each initial state we construct a series of tGGE density matrices of the form (4.16) and compute local correlators as a function of the series index n . For the truncation numbers we choose $N_s = N_d = n$. This is a simple practical choice, and other possibilities could be considered as well.

For each initial state we compute the physical root and hole densities from the mean values of the conserved charges by the relation (3.17). The generating function for the charges is obtained using the methods of [15, 24]. Having obtained the exact root densities we compute the source terms $\delta_s(u)$ of the fictitious TBA equations (4.18). Finally we build a series of TBA equations of the form (4.14) such that the source terms approximate the true source terms $\delta_s(u)$.

First we consider the set of functions $D = \{d(u), d'(u), d''(u), \dots\}$ and perform a Gram-Schmidt orthogonalization with respect to L_2 norm to obtain the set $\tilde{D} = \{\tilde{d}_j(u)\}_{j=1, \dots, \infty}$ described in the previous section. All source terms are even with respect to parity reversal, therefore in practice it is enough to consider the set $D_e = \{d(u), d''(u), d''''(u) \dots\}$. Then we project the functions $\delta_s(u)$ onto the space spanned by the first N elements of the set \tilde{D} :

$$\delta_s = \delta_s^{(n)} + \dots, \quad \delta_s^{(n)} = \sum_{k=1}^n \tilde{\beta}_{s,k} \tilde{d}_k,$$

where the dots represent the part of δ_s belonging to the remaining subspace of D_e . At each step we numerically solve the tGGE-TBA equations with the sources $\delta_s^{(n)}$ and evaluate the local correlation functions. These are then compared to the physical correlators, as obtained from the physical root densities and the long-time limit of the real time simulations.

For the numerical solution of the TBA the infinite system (4.25) has to be truncated to N_{eq} equations. In our calculations we chose N_{eq} big enough so that the final numerical results do not change more than $\mathcal{O}(10^{-8})$ as we increase N_{eq} further. We observed that for higher truncation in the tGGE (when there are accurate source terms present for higher strings as well) N_{eq} could be set to lower values. This is in accordance with our general conjecture that the asymptotics of the TBA for high string indices becomes irrelevant as soon as the lower nodes acquire the correct source terms.

5.1 The dimer state

The dimer state is a two-site product state where each block is a local singlet:

$$|D\rangle = \otimes_{j=1}^{L/2} \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}.$$

In this work we will use the zero-momentum projection, which is defined as

$$|D_0\rangle = \frac{1}{\sqrt{2}}(|D\rangle + U|D\rangle),$$

where U is the one-site translation operator.

This state has been studied extensively. Its overlaps with Bethe states were already calculated in [20], mean values of the ultra-local conserved charges were calculated in [16], and the

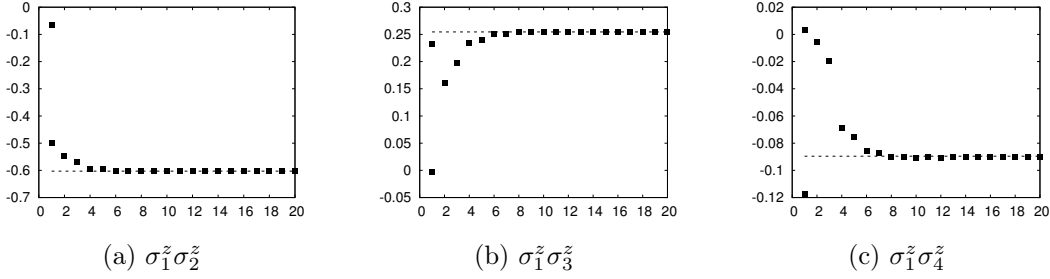


Figure 2: Evaluation of a few local observables within the truncated GGE for the dimer quench. The correlators $\sigma_1^z \sigma_a^z$, $a = 2, 3, 4$ are plotted as a function of the truncation index n . At each truncation step a total of $N_s N_d = n^2$ charges are included in the tGGE. The horizontal line shows the correlators computed using the Quench Action solution, which were shown to coincide with the asymptotics of the real time evolution [18]. The value of the anisotropy is $\Delta = 3$.

so-called Quench Action solution [19] was given in [18]. In [48] exact results were presented for the Y -functions using the methods of [47]. Furthermore, a complete analytic solution of the corresponding fusion hierarchy was given for the isotropic point $\Delta = 1$ in [51]. We note that for the dimer state the Y -functions satisfy the Y -system relations (4.8). In the works cited above this was assumed and also checked for the first few functions, whereas a general proof was later given in [49].

The source terms for the physical TBA are given explicitly by

$$\delta_s = -\log \frac{\vartheta_4^2}{\vartheta_1^2} + (-1)^s \log \frac{\vartheta_2^2}{\vartheta_3^2}, \quad (5.1)$$

where $\vartheta_{1,2,3,4}$ are Jacobi-functions with nome $e^{-2\eta}$ [47, 48]. As there are only two different source terms (for odd and even nodes), the approximation procedure for the sources can be done at the beginning only once, for δ_1 and δ_2 .

Examples for the local correlators as a function of the truncation index n are shown in Fig. 2. It can be seen that the physical values are obtained with big precision already around $n = 8$, which corresponds to adding $N_s N_d = n^2 = 64$ charges to the truncated GGE.

The approximation procedure gives us the Lagrange multipliers $\tilde{\beta}_{s,j}$ associated to the new set of charges. On the other hand, it is also useful to calculate the original n -dependent set $\beta_{s,j}(n)$ through relation (4.28). In Fig. 3 we plot the dependence of the first few Lagrange multipliers on the truncation index n . It can be seen that $\beta_{1,1}$ and $\beta_{2,1}$ (the first members of the $s = 1$ and $s = 2$ series) indeed tend to some well-defined values, as it was already explained in the previous section. However, $\beta_{1,2}$ and $\beta_{2,2}$ (which are the coefficients of the next charges in the respective series) are divergent. Similar behavior is observed for all $\beta_{s,j}$ with $j > 1$, therefore we did not plot further examples.

Fig. 4 shows how the approximation procedure works for the function $Y_1(u)$: the exact physical solution [48]

$$Y_1(u) = \frac{\cos(4\lambda) - \cosh(2\eta)}{\cos^2(\lambda)(\cos(2\lambda) - \cosh(\eta))} - 1$$

is compared to the solutions of the approximating TBA equations for the truncation numbers $n = 1, 6, 11$. The first figure shows $\log(Y_1(u))$ evaluated on the real line: indeed it can be observed that adding more and more charges gives a better approximation. However, the $\log(0)$ and $\log(\infty)$ singularities are never reproduced by the approximations, which are regular for each n . In contrast to this situation, the second figure shows the same function evaluated slightly off the real axis, for $u = x + 0.1i\eta$, where $x \in \mathbb{R}$. It can be seen that convergence is lost, and indeed our approximation procedure only works on the real line.

In the previous section it was remarked that the set of charges $\{Q_{s,j}\}$ is over-complete in the sense that a finite number of them can be omitted from the tGGE's and yet the correct

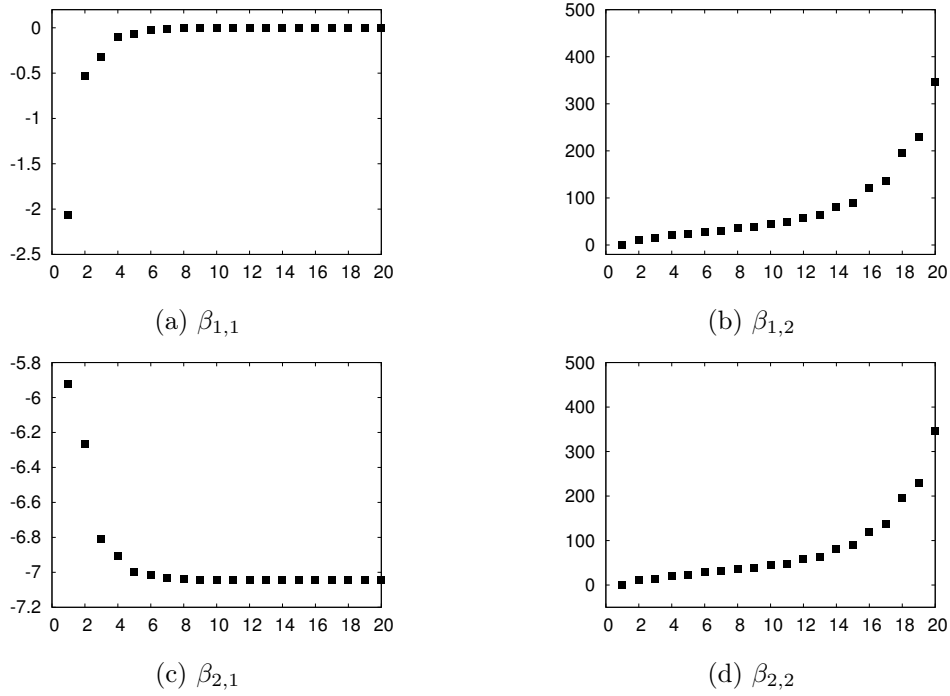


Figure 3: The dependence of the first few Lagrange multipliers $\beta_{s,j}$ on the truncation index n . For each spin index the first member $\beta_{s,1}$ tends to a constant value, while the remaining β 's are typically divergent.

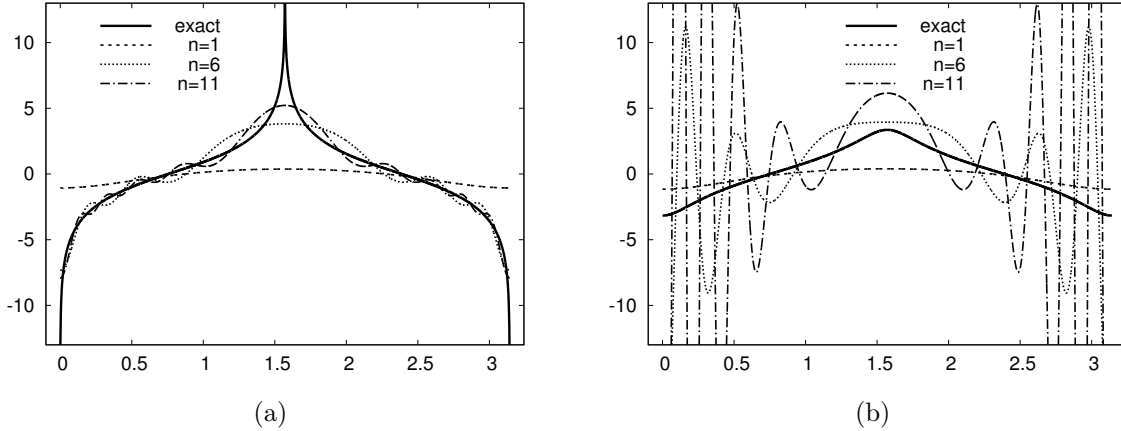


Figure 4: The function $\log(Y_1(u))$ of the dimer quench evaluated in the truncated GGE's together with the exact result. Fig. (a) shows the function for real u , whereas Fig. (b) is a plot of $\log(|Y_1(u)|)$ for $u = x + 0.1i\eta$ with $x \in \mathbb{R}$. The anisotropy is $\Delta = 3$.

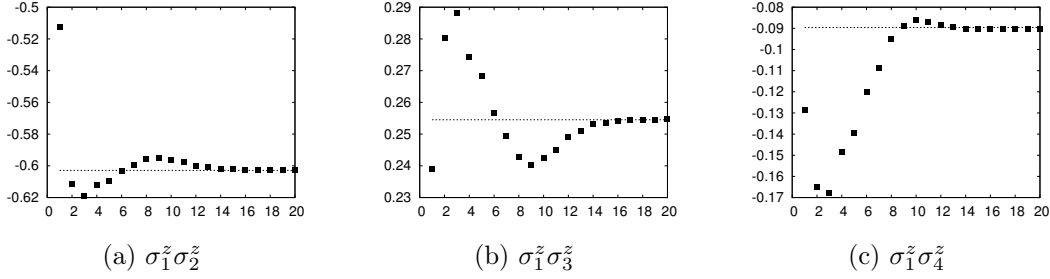


Figure 5: The $\sigma_1^z \sigma_a^z$ correlators within a defective tGGE with $a = 2, 3, 4$ for the dimer quench. Here $D = 3$. The defective GGE is built with the omission of the operators $Q_{s,2}$, which are the second charges for each spin/string index. Comparing with Fig. 2 it can be seen that the convergence in the truncation index is slower, but the physical correlators are reproduced nevertheless.

steady states can be reproduced. The only technical requirement is that the first members with $j = 1$ have to be included for each s . Here we numerically demonstrate this statement in the case of the dimer state. We build a defective tGGE where we leave out the second even charge for each string index. In terms of the TBA this corresponds to performing a Gram-Schmidt orthogonalization on the set $D' = D_e \setminus \{d''(u)\} = \{d(u), d^{(4)}(u), d^{(6)}(u), \dots\}$ and to use this basis to approximate the actual source terms. Numerical results for the correlators are depicted in Fig. 5. It can be seen that the correct values of the correlators are indeed reproduced, but the convergence is slower than in the case of the full tGGE's shown in Fig. 2.

5.2 Four-site states

Here we consider two different four site states as initial states. The first one is the domain wall state

$$|DW_4\rangle \equiv \otimes_{j=1}^{L/4} |\uparrow\uparrow\downarrow\downarrow\rangle.$$

This state has been already considered in [39], and exact expressions were derived for the root densities using the complete set of charges. Moreover, it was found that the resulting Y -functions do not satisfy the Y -system equations. Whereas it was already argued in [26] that this is the typical behavior for a quantum quench, real time evolution in such cases have not yet been considered in the literature.

We note that the domain wall state is similar to the Néel state in the sense that in the $\Delta \rightarrow \infty$ limit it becomes an exact eigenstate of the XXZ model. Therefore, it is expected that a quench from this initial state is a "small quench" for large and intermediate Δ , similar to what was observed for the Néel state in [17, 18].

In order to treat a four-site state with a certain degree of local entanglement we consider the initial state

$$|D_4\rangle = \otimes_{j=1}^{L/4} \frac{|\uparrow\uparrow\downarrow\downarrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle - |\uparrow\downarrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\downarrow\rangle}{2}.$$

It can be checked that in each four-site block the even and the odd sites are entangled with each other into an $SU(2)$ singlet. It follows that this state is $SU(2)$ invariant and it can be considered as resulting from a permutation of sites performed on the usual dimer state. Also, $|D_4\rangle$ is one of the ground states of the local Hamiltonian

$$H = J \sum_{j=1}^{L/4} (S_{4j} \cdot S_{4j+1} + S_{4j+1} \cdot S_{4j+3} + S_{4j+2} \cdot S_{4j+3} + S_{4j+2} \cdot S_{4j+4}) + \frac{J}{2} \sum_{j=1}^{L/2} (S_{2j} \cdot S_{2j+3} + S_{2j+1} \cdot S_{2j+2}).$$

This can be seen by performing a permutation of sites on the Majumdar-Ghosh Hamiltonian, for which the usual dimer state is an exact ground state.

In the case of the DW state the two-point correlators are two-site shift invariant, and for the generalized dimer there is only a four-site shift invariance. The GGE can only describe the zero momentum sector of the correlators. In order to compare the iTEBD data to the GGE we construct the averaged two-point functions

$$\langle \overline{\sigma_i^\alpha \sigma_{i+a}^\alpha} \rangle \equiv \sum_{j=1}^4 \langle \sigma_j^\alpha \sigma_{j+a}^\alpha \rangle, \quad a = 1, 2, \dots, \quad \alpha = x, y, z.$$

In Figs. 6 and 7 we plot the time evolution of short-range averaged z-z correlators against the prediction of the full micro-canonical ensemble. In the DW case we observe a relatively fast convergence, in accordance with this situation being a “small quench”. On the other hand, in the generalized dimer case the equilibration is considerably slower. It can be seen that the data does not contradict the GGE, but the time scales available to the iTEBD algorithm are too small to really confirm the predictions in this case. We note that plotting the individual correlators instead of the averaged ones we observe an even slower equilibration (even in the DW case), and our data is not sufficient to determine whether translational invariance is restored in the long time limit. We remind the reader that this is an open issue which to our best knowledge has not been resolved even for the simple two-site states [16, 18, 48].

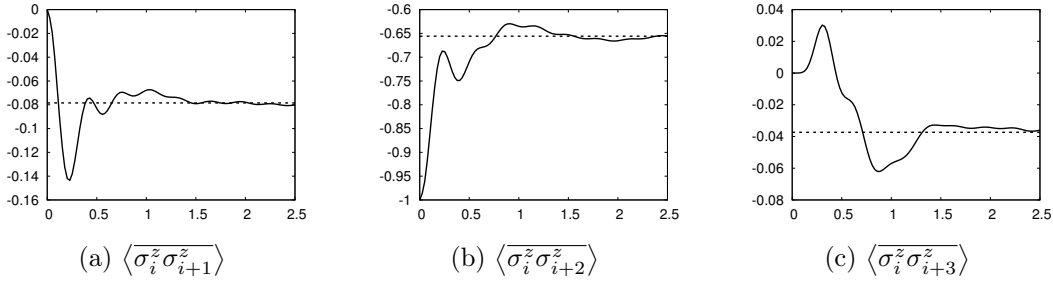


Figure 6: Time evolution of the averaged short range correlators in the quench starting from the 4-site DW state. The horizontal line is the prediction of the microcanonical GGE.

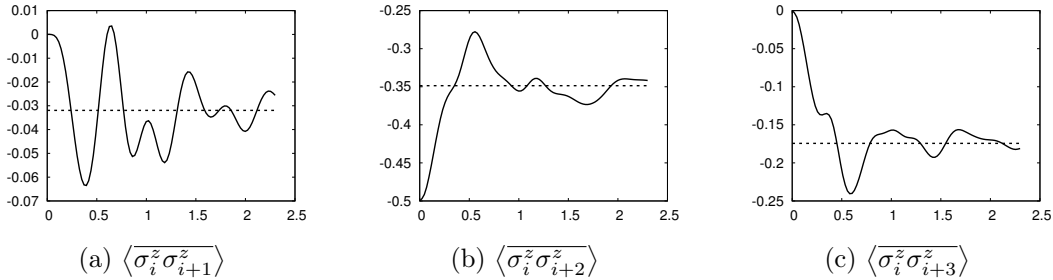


Figure 7: Time evolution of the averaged short range correlators in the quench starting from the generalized 4-site dimer state. The horizontal line is the prediction of the microcanonical GGE.

Figures 8 and 9 show the correlators evaluated within the tGGE’s for the DW and generalized dimer states, respectively. In both cases a fast convergence is observed. A remarkably good agreement with the full microcanonical ensemble is achieved already for $n = 4$, which corresponds to adding 16 charges to the tGGE.

6 Conclusions

In this work we re-considered the question whether a canonical Generalized Gibbs Ensemble can describe steady states after quenches in the XXZ chain. Instead of requiring

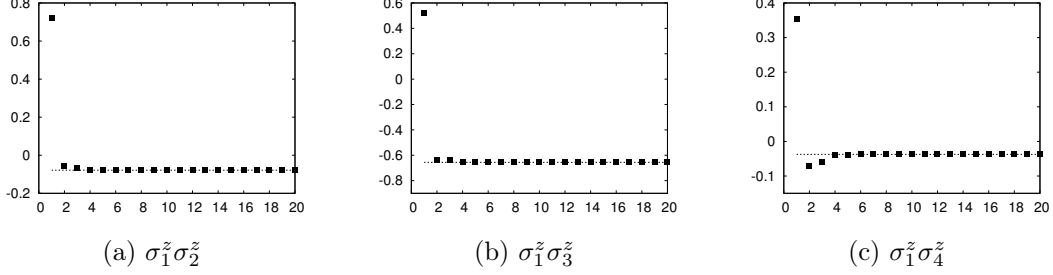


Figure 8: Evaluation of a few local observables within the truncated GGE for the quench from the 4-site DW state. The correlators $\sigma_1^z \sigma_a^z$, $a = 2, 3, 4$ are plotted as a function of the truncation index n . At each truncation step a total of $N_s N_d = n^2$ charges are included in the tGGE. The horizontal lines show the prediction of the full microcanonical GGE. The value of the anisotropy is $\Delta = 3$.

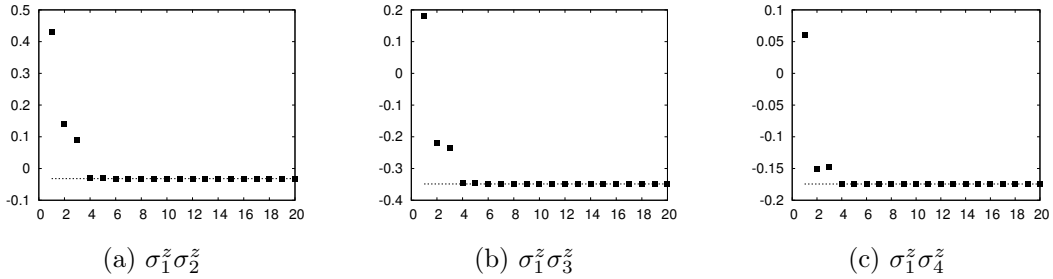


Figure 9: Evaluation of a few local observables within the truncated GGE for the quench from the 4-site generalized dimer state. The correlators $\sigma_1^z \sigma_a^z$, $a = 2, 3, 4$ are plotted as a function of the truncation index n . At each truncation step a total of $N_s N_d = n^2$ charges are included in the tGGE. The horizontal lines show the prediction of the full microcanonical GGE. The value of the anisotropy is $\Delta = 3$.

the definition of a GGE including all charges right from the start, we considered truncated GGE's with a finite number of discrete charges. Our goal was to show that the post-quench states can be approximated with arbitrary precision. To this order we constructed sequences of truncated GGE's, such that at each step only a finite number of ultra-local and quasi-local operators are included and the post-quench Bethe root densities (and therefore all local physical quantities) are exactly reproduced in the infinite truncation limit.

Our construction has a number of surprising properties. The GGE's are built using the canonical set of discrete charges, and we have shown that the associated Lagrange-multipliers are not well defined. In practice this means that as we add more and more charges to the GGE, the values of the first few Lagrange-multipliers need to be changed as well, and typically they diverge in the infinite truncation limit (except the first coefficients for each spin/string index). This means that they can not be considered physical state functions. The second striking property is that it is possible to omit a finite number of charges from the GGE, and the steady states can be reproduced nevertheless, although with a slower convergence of the tGGE.

Both of these problems can be overcome by constructing a new set of conserved operators, which is linearly related to the original set. We have shown that if the new set is chosen properly, the associated Lagrange-multipliers become well defined state functions, and they do not change as we add more and more operators. Conversely, none of the new charges can be omitted from the GGE. In this sense, the new set of charges plays a similar role as the Fourier modes of a free system.

These unexpected behaviors can be traced back to known mathematical facts about infinite dimensional vector spaces. Our initial goal was to approximate the exponent of the GGE density matrix using a discrete set of operators. In practice we have shown that the linear span of the canonical conserved charges is dense in the desired subspace of operators. However, in an infinite dimensional Banach space a set of vectors can be dense even when it is not a Schauder basis, i.e. when the expansion coefficients are not necessarily well defined. As an effect, the individual coefficients can oscillate or diverge even when the overall approximation is improving. And it is possible that some vectors can be omitted from the set such that the linear span will remain dense. However, after performing a Gram-Schmidt orthogonalization using an adequate inner product, the new set of vectors is guaranteed to be a Schauder basis: all expansion coefficients will be unique and none of the basis elements can be omitted from the set. We remark that in our construction the inner product for the Gram-Schmidt orthogonalization is not related to the original Hilbert space structure of the operators, instead it is derived from the Bethe Ansatz solution of the model (the norm is defined as the usual L_2 norm of the source functions for the TBA equations).

The physical conclusions to be drawn from our work are as follows. First of all, we would like to stress the physical relevance of the truncation of the GGE. In any physical situation one deals with a finite system, where only a finite number of charges are available. Moreover, in Section 5 we have shown that for given initial states it is enough to include only $\simeq 100$ charges, and all local correlators can be reproduced with remarkably good precision. Therefore, the truncated GGE has strong predictive power. On the other hand, we have also shown that if the set of conserved charges is chosen properly, all Lagrange-multipliers are finite, well defined, and they can be calculated using simple numerical procedures. Therefore, they are true physical state functions, that characterize the system.

It is important to compare our approach and results to those of [26]. The construction of [26] uses the particle number operators, which involve through formulas (4.9) and (4.10) the generating functions of the higher charges evaluated at an infinitesimally small distance from the boundary of the physical strip. The resulting operators are quasi-local for any finite value of the regulator, but they lose quasi-locality as this regulator is taken to zero. In contrast, our construction uses a discrete set of quasi-local operators such that the range of the operators is increased gradually. Nevertheless, the exponent of the tGGE is expected to lose the quasi-locality property in the infinite truncation limit. We stress that the physical observables are exactly reproduced by both approaches, and the difference lies only in the choice of

operators to approximate the exact GGE. Our method is built on the traditional requirement of statistical physics, namely that Gibbs or Generalized Gibbs Ensembles should be built using sufficiently local quantities, whereas the method of [26] provides a close connection to the particle picture, and to the GGE in free theories. We believe it would be useful to understand better the relation between the two approaches, and in particular the connection between the infinite truncation limit on one side, and the zero-regulator limit on the other.

Our results open the way for a number of further interesting questions.

It would be interesting to investigate which charges are the most relevant for the truncated GGE. In the present work we applied a simple procedure where at each truncation step we included the first n charges from the first n spin/string families. However, other schemes could be considered as well. This might shed light on how many discrete charges are actually needed to achieve a certain accuracy of the tGGE.

It would be useful to investigate quenches where the initial state is not a simple product state, for example the ground state of an other XXZ Hamiltonian. Our general derivation shows that the construction works for these states as well, and it would be interesting to see how the number of the required charges depends on the initial state.

Finally, it would be interesting to study truncated GGE's in other integrable models too. The essence of our construction, namely the technique of approximating the source terms of a TBA using a discrete set of charges is not limited to the XXZ chain. We expect similar behavior for other integrable models too, irrespective of their particle content. Note, that in our calculations the string structure of the TBA did not play a crucial role: the approximation procedure worked for each string index separately, resulting in the same linear transformation (4.27) for the charge families. Therefore, our construction is expected to work for various models which admit a TBA-like solution.

We hope to return to these questions in further research.

Acknowledgments

We are grateful to Jean-Sébastien Caux, Enej Ilievski, Márton Kormos, Izabella Lovas, Marko Medenjak, Lorenzo Piroli, Frank Pollmann, Tomaž Prosen, Eoin Quinn, Junji Suzuki and Gábor Takács for useful discussions. We are also thankful to Lorenzo Piroli for a careful reading of the manuscript. The proof of Theorem 1 was given by Christian Remling on Math.Stackexchange [50], and we are grateful to him for letting us use it. B. P. acknowledges support from the “Premium” Postdoctoral Program of the Hungarian Academy of Sciences, and the NKFIH grant no. K119204. E. V. acknowledges support from the ERC under Starting Grant 279391 EDEQS. M. W. acknowledges support from the NKFIH grants no. K105149 and SNN118028.

References

- [1] A. Polkovnikov, K. Sengupta, A. Silva, and M. Vengalattore, “*Colloquium* : Nonequilibrium dynamics of closed interacting quantum systems,” *Rev. Mod. Phys.* **83** (2011) 863–883, [arXiv:1007.5331 \[cond-mat.stat-mech\]](#).
- [2] J. Eisert, M. Friesdorf, and C. Gogolin, “Quantum many-body systems out of equilibrium,” *Nature Physics* **11** (2015) 124–130.
- [3] I. Bloch, J. Dalibard, and W. Zwerger, “Many-body physics with ultracold gases,” *Rev. Mod. Phys.* **80** (2008) 885–964.
- [4] M. A. Cazalilla, R. Citro, T. Giamarchi, E. Orignac, and M. Rigol, “One dimensional bosons: From condensed matter systems to ultracold gases,” *Rev. Mod. Phys.* **83** (2011) 1405–1466.

- [5] X.-W. Guan, M. T. Batchelor, and C. Lee, “Fermi gases in one dimension: From Bethe ansatz to experiments,” *Rev. Mod. Phys.* **85** (2013) 1633–1691.
- [6] M. T. Batchelor and A. Foerster, “Yang-Baxter integrable models in experiments: from condensed matter to ultracold atoms,” *Journal of Physics A: Mathematical and Theoretical* **49** (2016) no. 17, 173001, [arXiv:1510.05810 \[cond-mat.stat-mech\]](#).
<http://stacks.iop.org/1751-8121/49/i=17/a=173001>.
- [7] M. Rigol, V. Dunjko, V. Yurovsky, and M. Olshanii, “Relaxation in a Completely Integrable Many-Body Quantum System: An Ab Initio Study of the Dynamics of the Highly Excited States of 1D Lattice Hard-Core Bosons,” *Physical Review Letters* **98** (2007) no. 5, 050405, [arXiv:cond-mat/0604476](#).
- [8] M. Rigol, A. Muramatsu, and M. Olshanii, “Hard-core bosons on optical superlattices: Dynamics and relaxation in the superfluid and insulating regimes,” *Phys. Rev. A* **74** (2006) 053616, [arXiv:cond-mat/0612415](#).
- [9] C. Gramsch and M. Rigol, “Quenches in a quasidisordered integrable lattice system: Dynamics and statistical description of observables after relaxation,” *Phys. Rev. A* **86** (2012) 053615, [arXiv:1206.3570 \[cond-mat.stat-mech\]](#).
- [10] A. C. Cassidy, C. W. Clark, and M. Rigol, “Generalized Thermalization in an Integrable Lattice System,” *Physical Review Letters* **106** (2011) 140405, [arXiv:1008.4794 \[cond-mat.stat-mech\]](#).
- [11] F. H. L. Essler and M. Fagotti, “Quench dynamics and relaxation in isolated integrable quantum spin chains,” *Journal of Statistical Mechanics: Theory and Experiment* **6** (2016) 064002, [arXiv:1603.06452 \[cond-mat.quant-gas\]](#).
- [12] L. Vidmar and M. Rigol, “Generalized Gibbs ensemble in integrable lattice models,” *Journal of Statistical Mechanics: Theory and Experiment* **6** (2016) 064007, [arXiv:1604.03990 \[cond-mat.stat-mech\]](#).
- [13] T. Langen, S. Erne, R. Geiger, B. Rauer, T. Schweigler, M. Kuhnert, W. Rohringer, I. E. Mazets, T. Gasenzer, and J. Schmiedmayer, “Experimental observation of a generalized Gibbs ensemble,” *Science* **348** (2015) 207–211, [arXiv:1411.7185 \[cond-mat.quant-gas\]](#).
- [14] B. Pozsgay, “The generalized Gibbs ensemble for Heisenberg spin chains,” *Journal of Statistical Mechanics: Theory and Experiment* **2013** (2013) no. 07, 3, [arXiv:1304.5374 \[cond-mat.stat-mech\]](#).
- [15] M. Fagotti and F. H. L. Essler, “Stationary behaviour of observables after a quantum quench in the spin-1/2 Heisenberg XXZ chain,” *Journal of Statistical Mechanics: Theory and Experiment* **7** (2013) 12, [arXiv:1305.0468 \[cond-mat.stat-mech\]](#).
- [16] M. Fagotti, M. Collura, F. H. L. Essler, and P. Calabrese, “Relaxation after quantum quenches in the spin- $\frac{1}{2}$ Heisenberg XXZ chain,” *Physical Review B* **89** (2014) 125101, [arXiv:1311.5216 \[cond-mat.stat-mech\]](#).
- [17] B. Wouters, J. De Nardis, M. Brockmann, D. Fioretto, M. Rigol, and J.-S. Caux, “Quenching the Anisotropic Heisenberg Chain: Exact Solution and Generalized Gibbs Ensemble Predictions,” *Physical Review Letters* **113** (2014) no. 11, 117202, [arXiv:1405.0172 \[cond-mat.str-el\]](#).
- [18] B. Pozsgay, M. Mestyán, M. A. Werner, M. Kormos, G. Zaránd, and G. Takács, “Correlations after Quantum Quenches in the XXZ Spin Chain: Failure of the Generalized Gibbs Ensemble,” *Physical Review Letters* **113** (2014) no. 11, 117203, [arXiv:1405.2843 \[cond-mat.stat-mech\]](#).

- [19] J.-S. Caux and F. H. L. Essler, “Time Evolution of Local Observables After Quenching to an Integrable Model,” *Physical Review Letters* **110** (2013) no. 25, 257203, [arXiv:1301.3806 \[cond-mat.stat-mech\]](#).
- [20] B. Pozsgay, “Overlaps between eigenstates of the XXZ spin-1/2 chain and a class of simple product states,” *J. Stat. Mech.* **2014** (2014) no. 6, P06011, [arXiv:1309.4593 \[cond-mat.stat-mech\]](#).
- [21] K. K. Kozłowski and B. Pozsgay, “Surface free energy of the open XXZ spin-1/2 chain,” *J. Stat. Mech.* **2012** (2012) no. 05, 21.
- [22] M. Brockmann, J. De Nardis, B. Wouters, and J.-S. Caux, “A Gaudin-like determinant for overlaps of Néel and XXZ Bethe states,” *Journal of Physics A Mathematical General* **47** (2014) no. 14, 145003, [arXiv:1401.2877 \[cond-mat.stat-mech\]](#).
- [23] M. Brockmann, J. De Nardis, B. Wouters, and J.-S. Caux, “Néel-XXZ state overlaps: odd particle numbers and Lieb-Liniger scaling limit,” *ArXiv e-prints* (2014) , [arXiv:1403.7469 \[cond-mat.stat-mech\]](#).
- [24] E. Ilievski, J. De Nardis, B. Wouters, J.-S. Caux, F. H. L. Essler, and T. Prosen, “Complete Generalized Gibbs Ensembles in an Interacting Theory,” *Physical Review Letters* **115** (2015) no. 15, 157201, [arXiv:1507.02993 \[quant-ph\]](#).
- [25] E. Ilievski, M. Medenjak, T. Prosen, and L. Zadnik, “Quasilocal charges in integrable lattice systems,” *Journal of Statistical Mechanics: Theory and Experiment* **6** (2016) 064008, [arXiv:1603.00440 \[cond-mat.stat-mech\]](#).
- [26] E. Ilievski, E. Quinn, and J.-S. Caux, “From interacting particles to equilibrium statistical ensembles,” [arXiv:1610.06911](#).
- [27] M. Fagotti and F. H. L. Essler, “Reduced Density Matrix after a Quantum Quench,” *Physical Review B* **87** (2013) no. 24, 245107, [arXiv:1302.6944 \[cond-mat.stat-mech\]](#).
- [28] M. Kollar and M. Eckstein, “Relaxation of a one-dimensional Mott insulator after an interaction quench,” *Physical Review A* **78** (2008) no. 1, 013626, [arXiv:0804.2254 \[cond-mat.str-el\]](#).
- [29] M. Rigol, V. Dunjko, and M. Olshanii, “Thermalization and its mechanism for generic isolated quantum systems,” *Nature* **452** (2008) 854–858, [arXiv:0708.1324 \[cond-mat.stat-mech\]](#).
- [30] J. M. Deutsch, “Quantum statistical mechanics in a closed system,” *Physical Review A* **43** (1991) no. 4, 2046–2049.
- [31] M. Srednicki, “Chaos and quantum thermalization,” *Physical Review E* **50** (1994) 888–901, [arXiv:cond-mat/9403051](#).
- [32] A. C. Cassidy, C. W. Clark, and M. Rigol, “Generalized Thermalization in an Integrable Lattice System,” *Physical Review Letters* **106** (2011) no. 14, 140405, [arXiv:1008.4794 \[cond-mat.stat-mech\]](#).
- [33] S. Sotiriadis and P. Calabrese, “Validity of the GGE for quantum quenches from interacting to noninteracting models,” *Journal of Statistical Mechanics: Theory and Experiment* **2014** (2014) no. 7, P07024, [arXiv:1403.7431 \[cond-mat.stat-mech\]](#).
- [34] E. Ilievski, E. Quinn, J. De Nardis, and M. Brockmann, “String-charge duality in integrable lattice models,” *Journal of Statistical Mechanics: Theory and Experiment* **6** (2016) 063101, [arXiv:1512.04454 \[cond-mat.stat-mech\]](#).

- [35] A. De Luca, M. Collura, and J. De Nardis, “Non-equilibrium spin transport in the XXZ chain: steady spin currents and emergence of magnetic domains,” *ArXiv e-prints* (2016) , [arXiv:1612.07265](#) [[cond-mat.str-el](#)].
- [36] V. Korepin, N. Bogoliubov, and A. Izergin, *Quantum inverse scattering method and correlation functions*. Cambridge University Press, 1993.
- [37] M. Takahashi, *Thermodynamics of One-Dimensional Solvable Models*. Cambridge University Press, 1999.
- [38] E. Ilievski, M. Medenjak, and T. Prosen, “Quasilocal Conserved Operators in the Isotropic Heisenberg Spin-1/2 Chain,” *Physical Review Letters* **115** (2015) no. 12, 120601, [arXiv:1506.05049](#) [[cond-mat.stat-mech](#)].
- [39] L. Piroli, E. Vernier, and P. Calabrese, “Exact steady states for quantum quenches in integrable Heisenberg spin chains,” *Physical Review B* **94** (2016) no. 5, 054313, [arXiv:1606.00383](#) [[cond-mat.stat-mech](#)].
- [40] L. Piroli, E. Vernier, P. Calabrese, and M. Rigol, “Correlations and diagonal entropy after quantum quenches in XXZ chains,” *Phys. Rev. B* **95** (2017) 054308, [arXiv:1611.08859](#) [[cond-mat.stat-mech](#)].
- [41] C. N. Yang, “Some Exact Results for the Many-Body Problem in one Dimension with Repulsive Delta-Function Interaction,” *Physical Review Letters* **19** (1967) 1312–1315.
- [42] R. J. Baxter, *Exactly solved models in statistical mechanics*. London: Academic Press Inc, 1982.
- [43] M. Lüscher, “Dynamical charges in the quantized renormalized massive Thirring model,” *Nuclear Physics B* **117** (1976) no. 2, 475 – 492.
- [44] M. Takahashi, M. Shiroishi, and A. Klümper, “Equivalence of TBA and QTM,” *J. Phys. A* **34** (2001) no. 13, L187, [cond-mat/0102027](#).
- [45] M. Mestyán and B. Pozsgay, “Short distance correlators in the XXZ spin chain for arbitrary string distributions,” *Journal of Statistical Mechanics: Theory and Experiment* **9** (2014) 20, [arXiv:1405.0232](#) [[cond-mat.stat-mech](#)].
- [46] E. Vernier and A. C. Cubero, “Quasilocal charges and progress towards the complete GGE for field theories with nondiagonal scattering,” *Journal of Statistical Mechanics: Theory and Experiment* **2017** (2017) no. 2, 023101, [arXiv:1609.03220](#) [[cond-mat.stat-mech](#)]. <http://stacks.iop.org/1742-5468/2017/i=2/a=023101>.
- [47] M. Brockmann, B. Wouters, D. Fioretto, J. De Nardis, R. Vlijm, and J.-S. Caux, “Quench action approach for releasing the Néel state into the spin-1/2 XXZ chain,” *Journal of Statistical Mechanics: Theory and Experiment* **12** (2014) 12009, [arXiv:1408.5075](#) [[cond-mat.str-el](#)].
- [48] M. Mestyán, B. Pozsgay, G. Takács, and M. A. Werner, “Quenching the XXZ spin chain: quench action approach versus generalized Gibbs ensemble,” *Journal of Statistical Mechanics: Theory and Experiment* **4** (2015) 1, [arXiv:1412.4787](#) [[cond-mat.stat-mech](#)].
- [49] L. Piroli, B. Pozsgay, and E. Vernier, “From the Quantum Transfer Matrix to the Quench Action: The Loschmidt echo in XXZ Heisenberg spin chains,” *Journal of Statistical Mechanics: Theory and Experiment* **2017** (2017) no. 2, 023106.
- [50] C. Remling, “When does a real function together with its derivatives form a basis?.” Mathematics stack exchange. <http://math.stackexchange.com/q/876492>.

- [51] E. Ilievski, E. Quinn, J. De Nardis, and M. Brockmann, “String-charge duality in integrable lattice models,” *Journal of Statistical Mechanics: Theory and Experiment* **6** (2016) 063101, [arXiv:1512.04454](#) [`cond-mat.stat-mech`].
- [52] G. Vidal, “Efficient Classical Simulation of Slightly Entangled Quantum Computations,” *Physical Review Letters* **91** (2003) no. 14, 147902, [quant-ph/0301063](#).
- [53] G. Vidal, “Efficient Simulation of One-Dimensional Quantum Many-Body Systems,” *Physical Review Letters* **93** (2004) no. 4, 040502, [quant-ph/0310089](#).
- [54] G. Vidal, “Classical Simulation of Infinite-Size Quantum Lattice Systems in One Spatial Dimension,” *Physical Review Letters* **98** (2007) no. 7, 070201, [cond-mat/0605597](#).