Failure of the generalized eigenstate thermalization hypothesis in integrable models with multiple particle species

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Received 20 June 2014
Accepted for publication 25 July 2014
Published 22 September 2014

Abstract. It has been recently observed for a particular quantum quench in the XXZ spin chain that local observables do not equilibrate to the predictions of the generalized Gibbs ensemble (GGE). In this work we argue that the breakdown of the GGE can be attributed to the failure of the generalized eigenstate thermalization hypothesis (GETH), which has been the main candidate for explaining the validity of the GGE. We provide explicit counterexamples to the GETH and argue that generally it does not hold in models with multiple particle species. Therefore, there is no reason to assume that the GGE should describe the long time limit of observables in these integrable models.

Keywords: correlation functions, integrable spin chains (vertex models), thermodynamic Bethe Ansatz, quantum quenches

ArXiv ePrint: 1406.4613
1. Introduction

The problem of equilibration and thermalization of isolated quantum systems has received considerable interest over the last couple of years [1, 2]. One of the main questions is how the principles of statistical physics can be derived from the unitary time evolution of the quantum mechanical model. Interest in these questions has been sparked by new experimental techniques (for example with cold atoms [3]) where the systems are almost perfectly isolated from the environment and therefore equilibration induced by the system itself can be studied.

Equilibration in a quantum mechanical system means that the expectation values of physical observables are convergent as a function of time in the long time limit. Thermalization happens when these stationary values coincide with those obtained from a thermal ensemble. The full system never thermalizes as the unitary time evolution conserves all information about the initial state. On the other hand, the reduced density matrices of subsystems can approach their thermal values. Physically this means that the full system can act as a thermal bath for its subsystems and therefore expectation values of local observables indeed approach thermal predictions in the long time limit.

One of the main candidates for explaining why thermalization can happen is the eigenstate thermalization hypothesis (ETH) [4–6]. This states that in a typical interacting quantum system, the excited states that are close in energy have approximately the same
local correlation functions. Supplied with the assumption that in the long time limit dephasing between the eigenstates occurs, the ETH ensures that all local observables will approach thermal mean values with an effective temperature determined by the mean value of the energy in the initial state.

The situation is different in one-dimensional integrable models that possess a family of higher conserved charges, which prevent thermalization in the usual sense. It was proposed in [7] that correlation functions in integrable models approach values predicted by a generalized Gibbs ensemble (GGE), which incorporates all higher charges with appropriately chosen Lagrange multipliers. Furthermore it was proposed in [8] that equilibration to the GGE can be explained by a generalized eigenstate thermalization hypothesis (GETH). According to the GETH, the eigenstates that share the same set of conserved charges give approximately the same correlation functions. Both the GETH and the GGE are expected to become exact in the thermodynamic limit.

Since its inception, the idea of the GGE has become widely excepted in the field, partly because it was proven to be valid for models equivalent to free fermions [9–15]. However, it was found in [16] that for a certain quantum quench in the interacting spin-1/2 XXZ chain, the GGE gives different predictions than the quench action (QA) method [17], which (as opposed to the GGE) is built on first principles and is not based on any assumptions or approximations. Furthermore, clear evidence was found in a case of a different quench problem in [18] that while the predictions of the QA method coincide with results of real-time simulations, the GGE predictions are not correct. Differences between the GGE and real-time simulations had been observed in [19], but at that time they were interpreted as the result of very long relaxation times, which were beyond the reach of the simulations. However, the fact that the QA method (which is exact in the thermodynamic limit) correctly describes all local correlators [18] shows that it is the GGE itself that fails for these particular quench problems.

In [20] it was argued that the breakdown of the GGE can be explained by the fact that in Bethe ansatz solvable models with bound states, the set of higher conserved charges is not enough to determine the distribution of the pseudo-momenta of the particles. Therefore, states with different root distributions can share the same set of conserved charges, and still have different correlation functions. Examples for this had already been observed in [16], where it was shown that the QA method selects states that have the same conserved charges as the initial state, and still their correlation functions differ from the GGE predictions, even though the GGE states share the same set of charges by definition.

In the present work we take the argument of [20] further and show that the failure of the GGE can be attributed to the failure of the generalized eigenstate hypothesis in models with multiple particle species. For the XXZ spin chain, we develop a method to construct an arbitrary large family of eigenstates that share the same set of local conserved charges and still give different local correlations. We give explicit numerical examples for the failure of the GETH in the thermodynamic limit. It follows from our results that in a typical case the GGE cannot be a valid description of the long time limit behaviour of the system, irrespective of the initial state.

The article is organized as follows. In section 2 we introduce the concepts of thermalization, ETH, GGE and GETH. In section 3 we show that the GETH is not valid in the XXZ chain, and argue that this is a generic property of models with multiple particle species. In section 4 we provide explicit counterexamples of the GETH, which are related
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to a certain quantum quench problem. Section 5 includes our conclusions. Technical details for the calculation of correlation functions and the solution of the so-called thermodynamic Bethe ansatz (TBA) system with thermal asymptotics are presented in appendices A and B, respectively.

2. Thermalization in non-integrable and integrable models

Consider a generic local Hamiltonian $H$ in a finite volume $L$ with periodic boundary conditions. To be specific here we treat finite lattice models, but most of the arguments carry over to continuous models and field theories as well.

Consider the situation where at $t = 0$ the system is prepared in the initial state $|\Psi_0\rangle$ and for $t > 0$ it evolves unitarily with a local Hamiltonian $H$. Time-dependent expectation values of local observables are then computed as

$$\langle O(t) \rangle = \sum_{n,m} c_n c^*_m \langle m|O|n\rangle e^{-i(E_n - E_m)t},$$

where $c_n = \langle n|\Psi_0\rangle$. In the large time limit, by neglecting degeneracies we obtain the prediction of the so-called diagonal ensemble, where each state is weighted by the squared norm of its overlap with the initial state:

$$\lim_{t \to \infty} \langle O(t) \rangle = \sum_n |c_n|^2 \langle n|O|n\rangle.$$  \hfill (1)

In a finite system the limit in the left-hand side above does not exist and time averaging is required to obtain the diagonal ensemble on the right-hand side.

If the system is thermalized then in a large volume, all expectation values should be close to the canonical prediction

$$\langle O \rangle_T = \frac{\sum_n e^{-E_n/T} \langle n|O|n\rangle}{\sum_n e^{-E_n/T}},$$  \hfill (2)

with a temperature $T$ that is fixed by the requirement

$$\langle H \rangle_T = \langle \Psi_0|H|\Psi_0\rangle.$$

It is expected that (1) and (2) become equal in the thermodynamic limit.

The expressions (1) and (2) are seemingly unrelated, as the coefficients $|c_n|^2$ are typically random and do not coincide with the Boltzmann weights. However, it can be shown that in a large volume $L$ only those states that share the energy density of the initial state have a non-negligible overlap [6]:

$$E_n \approx \frac{\langle \Psi_0|H|\Psi_0\rangle}{L},$$  \hfill (3)

and that the width of the distribution of the energy density goes to zero in the thermodynamic limit at least as fast as

$$\Delta \left( \frac{E}{L} \right) = \frac{1}{L} \sqrt{\langle \Psi_0|H^2|\Psi_0\rangle - (\langle \Psi_0|H|\Psi_0\rangle)^2} \sim \frac{1}{\sqrt{L}}.$$  \hfill (4)
Equation (4) holds for local Hamiltonians and initial states $|\Psi_0\rangle$ that satisfy the cluster decomposition principle. Physically relevant states belong to this class.

The ETH [4–6] states that all eigenstates that are close in energy have almost the same expectation values of physical observables and therefore

$$
\sum_n |c_n|^2 \langle n | \mathcal{O} | n \rangle \approx \left( \sum_n |c_n|^2 \right) \langle n_1 | \mathcal{O} | n_1 \rangle = \langle n_1 | \mathcal{O} | n_1 \rangle,
$$

where it is enough to select one sample state $n_1$ that fulfils the condition (3) and $c_1 \neq 0$.

Applying the ETH to the ensemble average (2) we obtain that

$$
\langle \mathcal{O}_T \rangle \approx \langle n_1 | \mathcal{O} | n_1 \rangle,
$$

where we used that in a large volume the canonical ensemble also selects states that are close in energy, such that their energy density coincides with that of the initial state. Comparing (5) and (6) it follows that local observables indeed thermalize:

$$
\lim_{t \to \infty} \langle \mathcal{O}(t) \rangle \approx \langle \mathcal{O} \rangle_T.
$$

An exact equality is expected in the thermodynamic limit.

### 2.1. The GGE in integrable models

If the system is integrable then there exists a family of higher charges $\{Q_j\}$ such that each member is a sum of local operators and they all commute and the Hamiltonian is a member of the series. As a result the expectation values of the $Q_j$ are integrals of motion, which preclude thermalization in the usual sense. Nevertheless, even integrable models are expected to equilibrate and the question arises whether some kind of statistical physical ensemble describes the stationary values.

It was proposed in [7] that a GGE, which is the natural extension of the canonical ensemble, should describe the local observables. To be precise, the following should hold:

$$
\lim_{t \to \infty} \langle \mathcal{O}(t) \rangle = \langle \mathcal{O} \rho_{GGE} \rangle, \quad \text{where} \quad \rho_{GGE} = \frac{e^{-\sum j \lambda_j Q_j}}{\text{Tr} e^{-\sum j \lambda_j Q_j}},
$$

where the parameters $\lambda_j$ are fixed by the requirement

$$
\langle Q_j \rho_{GGE} \rangle = \langle \Psi_0 | Q_j | \Psi_0 \rangle, \quad j = 1 \ldots N_Q,
$$

where $N_Q$ is the number of the higher charges. In a finite volume we have typically $N_Q = L$.

Evidently it is necessary to add all existing local charges to the GGE. Also, it follows from the usual statistical physical arguments that only extensive operators can be added to the exponent, otherwise the thermodynamic limit could not be defined.

It was argued in [8] that a possible mechanism for thermalization in the GGE is the appropriate extension of the ETH to the integrable case: the GETH. This hypothesis states that if all local conserved charges of two different eigenstates are close to each other, then the mean values of all local operators are close too. In other words, the set of the conserved charges uniquely determines the correlations in the state, at least in the thermodynamic limit. For the diagonal ensemble this means that

$$
\lim_{t \to \infty} \langle \mathcal{O}(t) \rangle = \sum_n |c_n|^2 \langle n | \mathcal{O} | n \rangle \approx \left( \sum_n |c_n|^2 \right) \langle n_1 | \mathcal{O} | n_1 \rangle = \langle n_1 | \mathcal{O} | n_1 \rangle,
$$

doi:10.1088/1742-5468/2014/09/P09026
where we selected a sample state \( n_1 \) that fulfils the conditions \( c_1 \neq 0 \) and

\[
\frac{\langle n_1 | Q_j | n_1 \rangle}{L} \approx \frac{\langle \Psi_0 | Q_j | \Psi_0 \rangle}{L}, \quad j = 1 \ldots N_Q.
\]  

(10)

In (9), we assumed that only those states that fulfil the condition (10) have a non-negligible overlap. This follows from the fact the mean values of the charges are conserved in time, and the width of the distribution of the charge densities goes to zero according to

\[
\Delta \left( \frac{Q_j}{L} \right) = \frac{1}{L} \sqrt{\langle \Psi_0 | Q_j^2 | \Psi_0 \rangle - (\langle \Psi_0 | Q_j | \Psi_0 \rangle)^2} \sim \frac{1}{\sqrt{L}}.
\]  

(11)

Once again we used that the \( Q_j \) are sums of local operators and that \( | \Psi_0 \rangle \) satisfies the cluster decomposition principle.

By definition, the density matrix \( \rho_{\text{GGE}} \) generates states that have the prescribed charge densities, therefore applying the GETH again we obtain

\[
\langle O \rho_{\text{GGE}} \rangle \approx \langle n_1 | O | n_1 \rangle,
\]

and finally

\[
\lim_{t \to \infty} \langle O(t) \rangle \approx \langle O \rho_{\text{GGE}} \rangle.
\]  

(12)

The GETH has been checked for a lattice model of hard-core bosons in [8], but until recently it was an open question whether it holds in other integrable models. In this work we argue that in models with multiple particle species the GETH does not hold, and therefore in these cases there is no reason to assume that the system equilibrates to the GGE predictions.

3. The GETH in the XXZ spin chain

The most familiar interacting integrable models are the Bethe ansatz solvable theories [21]. A generic feature of these models is that the scattering processes are elastic and the multi-particle scattering processes factorize, i.e. they are products of two-particle scattering events. As a result multi-particle states are constructed using interacting single-particle wave functions, and interaction occurs only when two particles exchange positions [22]. In such models individual particles can be characterized by their particle type and their pseudo-momenta (rapidities). In the infinite volume limit and for finite particle density, it is possible to work with the rapidity distribution functions. It is a generic property of these models that in the thermodynamic limit the mean values of the local charges and also the correlation functions can be expressed using the rapidity distributions alone [16,21,23,24].

Here we argue, following [20], that in a theory with multiple particle types (whether fundamental particles or bound states), the GETH does not hold. The main reason for the failure of the GETH is that the countably infinite number of constraints posed by the local charges is not enough to fix the rapidity distributions if more than one particle is present in the spectrum. As a result, two different configurations can share the same charges, but yield different correlation functions.
As an example we consider the spin-1/2 XXZ chain defined by the Hamiltonian

$$H_{XXZ} = \sum_{j=1}^{L} \{ \sigma^x_j \sigma^x_{j+1} + \sigma^y_j \sigma^y_{j+1} + \Delta (\sigma^z_j \sigma^z_{j+1} - 1) \}. \quad (13)$$

We constrain ourselves to the regime $\Delta > 1$.

This model can be solved by the different forms of the Bethe ansatz [21]. Single-particle states are spin waves over the ferromagnetic reference state $|F+\rangle = |++...\rangle$. Multi-particle states can be formed by taking into account the factorized scattering between individual spin waves. The explicit wave function can be written as

$$\Psi_N(\lambda_1, \ldots, \lambda_N|s_1, \ldots, s_N) = \sum_{P \in \sigma_N} \prod_j \left( \frac{\sin(\lambda_{P_j} + i\eta/2)}{\sin(\lambda_{P_j} - i\eta/2)} \right)^{s_j} \prod_{j>k} \frac{\sin(\lambda_{P_j} - \lambda_{P_k} - i\eta)}{\sin(\lambda_{P_j} - \lambda_{P_k})}. \quad (14)$$

Here the variables $\lambda_j$ are the rapidities of the single spin waves, $s_j$ denote the positions of the down spins, and it is assumed that $s_j < s_k$ for $j < k$. The parameter $\eta$ is defined by $\Delta = \cosh(\eta)$. In a periodic system the rapidities are subject to the Bethe equations

$$\left( \frac{\sin(\lambda_j + i\eta/2)}{\sin(\lambda_j - i\eta/2)} \right)^L \prod_{k \neq j} \frac{\sin(\lambda_j - \lambda_k - i\eta)}{\sin(\lambda_j - \lambda_k + i\eta)} = 1. \quad (15)$$

The canonical set of commuting local charges of the theory $\{Q_j\}_{j=1..L}$ can be constructed using the algebraic Bethe ansatz [21]. Their eigenvalues for a multi-particle state are given by

$$Q_j |\{\lambda\}_N\rangle = \left( \sum_{k=1}^{N} q_j(\lambda_k) \right) |\{\lambda\}_N\rangle, \quad (16)$$

where

$$q_j(u) = -i \left( \frac{\partial}{\partial u} \right)^j \log \left( \frac{\sin(\lambda_j + i\eta/2)}{\sin(\lambda_j - i\eta/2)} \right). \quad (17)$$

The Hamiltonian itself is the first member of the series. To be more precise, in the present normalizations we have

$$H = 2 \sinh(\eta)Q_1. \quad (18)$$

If $\Delta \geq 1$ then spin waves can form arbitrary large bound states, which are called ‘strings’ [25]. For a bound state of $n$ fundamental spin waves the rapidities are arranged as

$$\{\lambda\} = x - \frac{n}{2} \frac{1}{2} + i\delta_1, x - \frac{n}{2} - \frac{3}{2} \frac{1}{2} + i\delta_2, \ldots, x + \frac{n}{2} \frac{1}{2} + i\delta_n.$$ 

The variable $x \in [-\pi/2, \pi/2]$ is the string centre and the $\delta_j$ are string deviations, which become exponentially small in the large volume limit. In the present context, it is useful to regard the different strings as different particle types.

In the thermodynamic limit it is convenient to introduce densities for the string centres such that in a volume $L$ the number of $k$-strings with centres between $\lambda$ and $\lambda + d\lambda$ is $L \rho_{r,k}(\lambda)/2\pi$. The magnetization of the system is then given by

$$\langle S^z \rangle = 1/2 - \sum_{k=1}^{\infty} k \int d\lambda \frac{\rho_{r,k}(\lambda)}{2\pi}. \quad (19)$$

doi:10.1088/1742-5468/2014/09/P09026
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It is also useful to introduce the densities \( \rho_{h,k}(\lambda) \) for the holes, which are the generalization of empty levels of a free theory to the Bethe ansatz solvable case. It can be derived from the Bethe equations that these functions satisfy the linear equations [25]

\[
\rho_{r,k} + \rho_{h,k} = \delta_{k,1} d + d \ast (\rho_{h,k-1} + \rho_{h,k+1}),
\]

where

\[
d(u) = 1 + 2 \sum_{n=1}^{\infty} \frac{\cos(2nu)}{\cosh(\eta n)} \tag{20}
\]

and the convolution of two functions is defined as

\[
(f \ast g)(u) = \int_{-\pi/2}^{\pi/2} \frac{d\omega}{2\pi} f(u - \omega)g(\omega). \tag{21}
\]

Instead of working with the individual conserved charges it is useful to define the generating function [26]

\[
G(\lambda) = \sum_{k=1}^{\infty} \frac{\lambda^{k-1}}{(k-1)!} \langle Q_k \rangle. \tag{22}
\]

It was shown in [16] that \( G(\lambda) \) can be expressed using \( \rho_{h,1}(\lambda) \) alone. With our conventions, the following equation holds:

\[
d \ast (s_1 + \rho_{h,1}) = G, \tag{23}
\]

where

\[
s_1 = -\sinh(\eta) \frac{\sin(\lambda + i\eta/2)}{\sin(\lambda - i\eta/2)}. \tag{24}
\]

Equation (23) means that different configurations that have the same \( \rho_{h,1} \) also share the same set of local conserved charges.

Local correlation functions for arbitrary string distributions can be computed using the method of [24], which uses results from the theory of factorization of correlation functions in the finite temperature case [27,28].

For generic string distributions, we propose regarding the hole densities \( \{\rho_{h,k}\}_{k=1,\ldots,\infty} \) as the fundamental variables describing the states. This has the advantage that the root densities are easily obtained from (19) by a simple convolution without the need to solve any linear equations. Moreover, all local correlators can be computed from the hole densities using the following steps:

- As a first step compute the root densities \( \{\rho_{r,k}\}_{k=1,\ldots,\infty} \) from (19). For each string type calculate the functions

\[
\eta_k(\lambda) = \frac{\rho_{h,k}(\lambda)}{\rho_{r,k}(\lambda)}.
\]

- Use the functions \( \eta_k(\lambda) \) as an input to certain linear equations for two series of auxiliary functions \( \rho_k^{(a)} \) and \( \sigma_k^{(a)} \), where \( a = 0, \ldots, \infty \) and \( k \) is the string index.

- Compute the local correlators using certain integrals over the auxiliary functions.

1 Although at present the main results of [24] are only conjectures, they have been verified numerically in the finite temperature case [24] and also for a non-trivial quench problem in [18].
The details of this procedure can be found in appendix A, which includes new and more efficient formulas compared to those of [24].

We stress that while the local charges only depend on ρ_{h,1}, the correlations depend on all ρ_{h,k}. On a technical level this is why the GETH fails: fixing ρ_{h,1} leaves the functions ρ_{h,k} with k > 2 arbitrary and therefore the local correlators are not specified by the charges only.

To conclude this section, we point out a simple relation between the hole densities and the overall magnetization. Multiplying the k-th equation of (19) with k, integrating over the rapidity and summing over k we obtain

\[ \langle S_z \rangle = \frac{1}{2} - \lim_{k \to \infty} \left( k \sum_{j=1}^{k} \int \rho_{r,j} \right) = \frac{1}{2} \lim_{k \to \infty} \left( (k - 1) \int \rho_{h,k} \frac{1}{2\pi} - k \int \rho_{h,k+1} \frac{1}{2\pi} \right). \]

Therefore the total magnetization is zero for arbitrary hole densities as long as the limit on the right-hand side above vanishes.

4. Examples of the failure of the GETH

In this section we treat a specific quantum quench problem and explicitly demonstrate the failure of the GETH in this case. The problem we consider is the quench from the Majumdar–Ghosh dimer state, i.e. we assume that at t = 0 the system is prepared in the translationally invariant combination

\[ |Ψ(t=0)⟩ = \frac{1}{\sqrt{2}}(1 + T) \left[ ⊗^{L/2} |+⟩ - |−⟩ \right] \left[ ⊗^{L/2} |+⟩ - |−⟩ \right], \]

where T is the translation operator for one site. This vector is one of the ground states of the Majumdar–Ghosh Hamiltonian [29].

This particular quench problem has already been considered in the works [19] and [18], both of which included numerical results from real-time simulations. In [19] the GGE predictions for local observables were calculated using the quantum transfer matrix (QTM) method (see also [26,30]). Although discrepancies were found between the GGE and the real-time simulations, they were interpreted as a result of long relaxation times. On the other hand, the exact predictions from the quench action (QA) method were computed in [18] and they were found to agree with the real-time data. Therefore it was concluded in [18] that it is the GGE which is not correct in this case.

In section 4.1 we recall the QA solution of this quench problem. In section 4.2 we provide the GGE predictions using the TBA method and show that they agree with the numerical results of [19]. Finally in section 4.3 we develop a method to generate root configurations that have the same conserved charges but different correlators and thus demonstrate the failure of the GETH.

The paper [19] considered a single dimer product state and not the translational invariant combination. In this case it is a separate question whether translational invariance is restored in the long time limit. However, the GGE was supposed to describe the averaged correlators, whereas the numerical evidence in both [19] and [18] shows that it fails to do so.

doi:10.1088/1742-5468/2014/09/P09026
4.1. The quench action solution

The QA method developed in [17] is an exact method (in the thermodynamic limit), which selects the eigenstates that dominate the dynamics of the system in the long time limit. It does so by minimizing the so-called QA, which is the combination of the exact overlaps and the micro-canonical entropy associated with each state. For the XXZ chain, the main steps of the solution are as follows.

In a large volume, the summation over the states in the diagonal ensemble (1) can be replaced by a functional integral over the densities. In accordance with the proposal in the previous section, we regard the hole densities as the basic variables and write

\[ \lim_{t \to \infty} \langle \mathcal{O}(t) \rangle = \int \prod_{j=1}^{\infty} \mathcal{D}(\rho_{h,j}(\lambda)) \langle \{\rho_h\}|\mathcal{O}|\{\rho_h\}\rangle e^{-LS[\{\rho_h\}]}, \]  

(26)

where \( S[\{\rho_{h,j}\}] \) is the QA. If the exact finite volume overlaps can be written as

\[ |\langle \Psi_0(\lambda) N \rangle|^2 = C \prod_{j=1}^{N} v(\lambda_j), \]

where \( C = \mathcal{O}(L^0) \), then the QA is expressed as

\[ S[\{\rho_{h,j}\}] = -\sum_{j=1}^{\infty} \int_{-\pi/2}^{\pi/2} \frac{du}{2\pi} \left( \rho_{r,j}(\lambda)g_j(\lambda) + \frac{1}{2}s_j(\lambda) \right), \]  

(27)

where the \( g_j \) and \( s_j \) are the overlap and entropy terms for the \( j \)-strings:

\[ g_j(\lambda) = \sum_{k=1}^{j} \log \left( v(\lambda + i\eta(n + 1 - 2k)/2) \right) \]  

(28)

\[ s_j(\lambda) = \rho_{r,j}(\lambda) \log \left( \frac{\rho_{r,j}(\lambda) + \rho_{h,j}(\lambda)}{\rho_{r,j}(\lambda)} \right) + \rho_{h,j}(\lambda) \log \left( \frac{\rho_{r,j}(\lambda) + \rho_{h,j}(\lambda)}{\rho_{h,j}(\lambda)} \right), \]  

(29)

and it is understood that the root densities are calculated from the hole densities using (19). The factor of 1/2 in front of the entropy in (27) takes into account that the exact overlaps are non-zero only if the state is exactly parity symmetric, i.e. it consists of rapidity pairs \( \{\pm \lambda\} \) [31,32]. Exact overlaps were calculated for the Néel initial state in [31,33]. For the dimer state it was obtained in [18] using the results of [33,34] that

\[ v(\lambda) = \frac{\sinh^4(\eta/2) \cot^2(\lambda)}{\sin(\lambda + 2i\eta) \sin(\lambda - 2i\eta)}. \]

The expression (26) is evaluated for the saddle point approximation, which is exact in the thermodynamic limit. Local operators do not shift the position of the saddle point, which is therefore obtained by the minimization of the quench action itself. The appropriate generalization of the TBA method [25] leads to the following set of equations for \( \eta_j = \rho_{h,j}/\rho_{r,j} \) [16]:

\[ \log \eta_j = f_j + d \star [\log(1 + \eta_{j-1}) + \log(1 + \eta_{j+1})], \]  

(30)

where

\[ f_j = -g_j + d \star (g_{j-1} + g_{j+1}), \text{ with } g_0 = 0. \]  

(31)
Having found the solution of (30), the string densities are calculated from (19) and correlators can be computed using the method described in [24] and appendix A. This task was performed in [18] for different values of $\Delta$ and the QA predictions were found to be in perfect agreement with the results of real-time simulations\(^3\). Also, it was found that the saddle point solution $\{\rho_{QA}^{h,j}\}$ yields the correct local charges and that

$$S'[\{\rho_{h,j}\}] = 0.$$  

(32)

The vanishing of the QA at the saddle point solution is a very strong physical requirement, which follows from the normalization of the initial state [18]:

$$1 = \langle \Psi_0 | \Psi_0 \rangle = \int \prod_{j=1}^{\infty} D(\rho_{h,j}(\lambda)) \ e^{-LS[\rho_{h,j}]}.$$  

(33)

It follows from (33) that any root distribution that yields a positive QA has zero spectral weight in the $L \to \infty$ limit and therefore it is irrelevant for the dynamics of the system.

### 4.2. The GGE-TBA predictions

Here we provide the TBA solution of the GGE for the quantum quench from the dimer state. The goal is to compute the local observables from the GGE as

$$\langle O_{GGE} \rangle = \frac{\text{Tr}(O e^{-\sum_j \lambda_j Q_j})}{\text{Tr}(e^{-\sum_j \lambda_j Q_j})}. \quad (34)$$

The standard treatment of the TBA method selects states with particle distributions $\rho_{r,k}$ and $\rho_{h,k}$ that minimize the generalized free energy obtained from the generalized Boltzmann weights. The following equation is obtained for the functions $\eta_k$ [16]:

$$\log \eta_j = \delta_{j,1} \left( -\sum_{k=1}^{\infty} \lambda_k d(k^{-1}) \right) + d \ast [\log(1 + \eta_{j-1}) + \log(1 + \eta_{j+1})],$$  

(35)

where

$$d^{(a)}(u) = \left( \frac{\partial}{\partial u} \right)^a d(u)$$

and $d(u)$ is given by (20). The Lagrange multipliers should be fixed by the requirement that the solution of (37) together with the equation for the densities (19) yields the correct local charges. It follows from (23) that it is enough to fix the function $\rho_{h,1}$ and this can be used to solve the GGE-TBA without the parameters $\lambda_j$ [16]. The details of this method were not given in [16], therefore we describe the method that we used.

The two system of equations (35) and (19) can be considered simultaneously. From the first equation in (19), we obtain

$$\rho_{h,1}(1 + 1/\eta_1) = d + d \ast \frac{\rho_2}{1 + 1/\eta_2}. \quad (36)$$

\(^3\) A different form of the overlap-TBA equations was used in [18] where all equations were coupled and a Lagrange multiplier fixing the overall magnetization was present. However, the two formulations lead to the same numerical results [35].
Assuming that $\rho_{h,1}$ is known we can take $\eta_1$ from this equation and substitute it into the second equation in (35). This way we obtain the following closed set of equations:

$$\log \eta_2 = d \ast \left[ \log \left( \frac{d + d \ast \frac{\rho_2}{1 + \frac{1}{\eta_2}}}{d + d \ast \frac{\rho_2}{1 + \frac{1}{\eta_2}} - \rho_{1,h}} \right) + \log(1 + \eta_3) \right]$$

$$\rho_2 = d \ast \left[ \eta_1 + \frac{\rho_3}{1 + \frac{1}{\eta_3}} \right]$$

$$\log \eta_j = d \ast \left[ \log(1 + \eta_{j-1}) + \log(1 + \eta_{j+1}) \right], \quad j > 2$$

$$\rho_j = d \ast \left[ \frac{\rho_{j-1}}{1 + \frac{1}{\eta_{j-1}}} + \frac{\rho_{j+1}}{1 + \frac{1}{\eta_{j+1}}} \right], \quad j > 2.$$  

These equations can be solved numerically by a simultaneous iteration, which we found to converge very well (in particular no damping of the iterations was required). Once the solution is found the correlators can be computed using the method described in appendix A.

It is useful to consider the asymptotic behaviour of the solution of the GGE-TBA, which is the same as in the purely thermal case. For large $j$ the $\eta_j(u)$ become approximately constant functions. Therefore we obtain the algebraic equations

$$\eta_j^2 = (1 + \eta_{j-1})(1 + \eta_{j+1}).$$  

The general solution at zero magnetization is [25]

$$\eta_j = (j + a)^2 - 1,$$  

where $a$ is an arbitrary real number. At infinite temperature (or equivalently if all $\beta_j$ of the GGE vanish), equation (38) is valid at arbitrary $j$ and we obtain $a = 1$. On the other hand, at zero temperature ($\beta_1 = \infty$), we obtain the ground state, which consists of 1-strings only with no holes and therefore $a = 0$. In the general case $a$ depends on all of the Lagrange multipliers.

For higher strings, the density functions also become rapidity independent and the total densities $\rho_j = \rho_{v,j} + \rho_{h,j}$ satisfy

$$\rho_j = \frac{1}{2} \left( \rho_{j-1} \frac{(j - 1 + a)^2 - 1}{(j - 1 + a)^2} + \rho_{j+1} \frac{(j + 1 + a)^2 - 1}{(j + 1 + a)^2} \right).$$

The physically relevant, decaying solution to this equation is

$$\rho_j = \frac{\alpha}{(j + a)^2 - 1},$$

where $\alpha$ depends on the particular situation. With the help of equations (39) and (41), a very efficient iteration scheme can be constructed, which produces highly accurate numerical results such that only a small number of equations is kept from the infinite system (37). Details of this method are described in appendix B.

In the dimer case, the generating function for the charges was calculated in [19]. In our normalizations it reads

$$G_D = - \sinh(\eta) \frac{4 \cos(2\lambda)(\sinh^2(\eta) - \cosh(\eta)) + \cosh(\eta) + 2 \cosh(2\eta) + 3 \cosh(3\eta) - 2}{4(\cosh(2\eta) - \cos(2\lambda))^2}.$$  

doi:10.1088/1742-5468/2014/09/P09026

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Table 1. The GGE predictions for short-range $z\rightarrow z$ correlators for the quench starting from the dimer state.

| $\Delta$ | $\langle \sigma^z_1 \sigma^z_2 \rangle$ | $\langle \sigma^z_1 \sigma^z_3 \rangle$ | $\langle \sigma^z_1 \sigma^z_4 \rangle$ |
|---------|--------------------------------|--------------------------------|--------------------------------|
| 1.4     | $-0.558 339 3723$             | $0.253 104 6021$             | $-0.142 796 7954$             |
| 1.6     | $-0.575 094 1519$             | $0.279 314 0206$             | $-0.157 465 2764$             |
| 2       | $-0.591 897 2433$             | $0.307 962 7101$             | $-0.165 265 1609$             |
| 3       | $-0.594 324 5488$             | $0.317 065 6703$             | $-0.140 569 0303$             |
| 4       | $-0.584 162 0734$             | $0.304 496 3585$             | $-0.111 778 6185$             |
| 5       | $-0.573 904 3321$             | $0.290 896 2124$             | $-0.090 028 9420$             |

Inverting the convolution (23), we obtained

$$\rho_{1,\text{hole}} + s_1 = -\frac{D}{2} (s_1 + s_3) + \frac{C}{2} (\bar{s}_1 + \bar{s}_3),$$

where

$$s_3(u) = -\frac{\sinh(3\eta)}{\sin(u + 3i\eta/2) \sin(u - 3i\eta/2)}$$

$$\bar{s}_1(u) = -\frac{1}{2} \left( \frac{1}{\sin^2(u + i\eta/2)} + \frac{1}{\sin^2(u - i\eta/2)} \right)$$

$$\bar{s}_3(u) = -\frac{1}{2} \left( \frac{1}{\sin^2(u + 3i\eta/2)} + \frac{1}{\sin^2(u - 3i\eta/2)} \right)$$

and

$$D = -\frac{\sinh(\eta)}{4 \sinh^3(2\eta)} \left( \frac{3}{2} \cosh(5\eta) + \cosh(4\eta) + \frac{1}{2} \cosh(3\eta) - 2 \cosh(\eta) - 1 \right)$$

$$C = -\frac{\sinh(\eta)}{4 \sinh^2(2\eta)} \left( \cosh(4\eta) + \cosh(3\eta) - \cosh(\eta) - 1 \right).$$

We substituted (43) into (37) and computed numerical results for short-range correlators for various values of $\Delta$. Examples of the results are given in table 1. Our numerical results agree with those obtained in [19] and they differ from the QA predictions [18].

It is interesting to consider the QA evaluated at the GGE saddle point, which gives information about its spectral weight in (26) and therefore its relevance for the quench dynamics\(^4\). If a non-zero value of the QA is found then this alone proves that the GGE cannot describe the asymptotic steady state of the system. Quite surprisingly an even stronger result holds: in this particular quench problem the QA is infinite for any configuration where the root densities have thermal asymptotes for higher strings, and this includes the GGE solution. Our statement follows from the fact that for large $j$ we have

$$\rho_{r,j} = \frac{\rho_{r,j} + \rho_{h,j}}{1 + \eta_j} \sim \frac{1}{j^3},$$

and the large $j$ asymptote of the overlap source is [18]

$$g_j \approx -\eta_j^2.$$\(^4\)

The idea to evaluate the QA for the GGE solution was suggested to us by Márton Mestyán.

\(^4\) doi:10.1088/1742-5468/2014/09/P09026
It is easy to see that the entropy is finite, therefore the overlap terms make expression (27) infinite if the asymptote (46) holds. The physical meaning of this finding is that the spectral weight of these states in (1) decays faster than exponentially as a function of the volume. We note that the same behaviour is found for the quantum quench starting from the Néel state.

4.3. Generating new configurations

The discrepancy between the predictions of the QA and GGE-TBA methods is already a sign of the failure of the GETH. Both methods give the same set of local charges, and therefore they share the hole density for the 1-strings. However, the other hole densities \( \rho_{h,j}, j > 2 \), are different and therefore the correlation functions are different. This phenomenon was observed in [16] for the quantum quench starting from the Néel state.

Here we show that an arbitrary large family of configurations can be generated that share the mean values of the charges but can have arbitrary correlation functions. The easiest way to construct new states is by altering the hole densities themselves. For example we can start with the QA solution \( \{\rho_{QA_{h,j}}\} \) and modify a handful of the hole densities, calculate the new root densities from (19) and the correlators from the formulas in appendix A. Alternatively one could interpolate between the QA and GGE solutions as

\[
\rho_{h,j}(\beta) = (1 - \beta)\rho_{QA_{h,j}} + \beta\rho_{GGE_{h,j}}, \quad \text{where} \quad \beta = 0, \ldots, 1,
\]

such that all correlations would interpolate between their QA and GGE values.

For our numerical examples, we choose a similar but numerically more convenient method. We consider an artificial modification of the GGE-TBA system (37) such that we add new source terms to a finite number of the equations. The sources can be arbitrary functions, but we chose the functions that appear in the overlap-TBA (30). This way we obtain configurations that share the thermal asymptotes but whose correlation functions can be arbitrarily close to those of the QA saddle point. For the numerical calculations we considered the equations

\[
\log \eta_2 = \beta_2 f_2 + d \ast \left[ \log \left( \frac{d + d \ast \rho_2}{1 + 1/\eta_2} \right) + \log(1 + \eta_3) \right]
\]

\[
\rho_2 = d \ast \left[ \rho_{1,h} + \frac{\rho_3}{1 + 1/\eta_3} \right]
\]

\[
\log \eta_j = d \ast \left[ \log(1 + \eta_{j-1}) + \log(1 + \eta_{j+1}) \right], \quad j > 2
\]

\[
\rho_j = d \ast \left[ \frac{\rho_{j-1}}{1 + 1/\eta_{j-1}} + \frac{\rho_{j+1}}{1 + 1/\eta_{j+1}} \right], \quad j > 2.
\]

Here a new source term is added only to the equation for \( \eta_2 \). The function \( f_2 \) is the source of the overlap-TBA defined in (31), and \( \beta_2 \) is an arbitrary real number. At \( \beta_2 = 0 \) we obtain the GGE solution, whereas for \( \beta_2 = 1 \) the resulting densities (for small \( j \)) are more similar to the solution of the overlap-TBA. Note that by gradually adding all higher source terms \( f_j \), a point-wise convergence to the overlap-TBA solution could be achieved. Surprisingly, the addition of \( f_2 \) results in correlators that are similar to the exact QA predictions. Numerical results as a function of \( \beta_2 \) are shown in figure 1.

doi:10.1088/1742-5468/2014/09/P09026
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Figure 1. (a) $\langle \sigma_i^z \sigma_j^z \rangle$, (b) $\langle \sigma_i^z \sigma_3^z \rangle$. Examples for short-range correlators for $\Delta = 3$ as a function of $\beta_2$, which is the coupling of the artificial source term in (47). The data points correspond to different root configurations that have the same conserved charges as the dimer initial state but different local correlations. The dashed and the dotted lines correspond to the GGE and QA predictions, respectively. The former were obtained from the GGE-TBA system (37), whereas the latter were taken from [18]. The point $\beta_2 = 0$ corresponds to the GGE solution, whereas at $\beta_2 = 1$ the correlators are close, but not identical to the QA prediction. The numerical data refer directly to the thermodynamic limit, therefore they directly demonstrate the failure of the GETH.

5. Conclusions

In this work we demonstrated that the GETH is not valid in the XXZ spin chain. Following [20], it can be argued that the GETH breaks down in all models with multiple particle species. As a result, the GGE does not give correct predictions for the stationary values of local correlators. This follows from the fact that the squared overlaps, which are the statistical weights in the diagonal ensemble, are unrelated to the generalized Boltzmann weights of the GGE, and if the GETH fails, the states selected by the two ensembles typically yield different correlation functions. In fact, in the absence of the GETH it would be an exception to find examples where the GGE would predict the correct stationary state. It is important to stress that all our results refer directly to the infinite volume limit and therefore there are no finite size effects to be considered.

On a technical level, we argued that in the XXZ spin chain the hole densities of the strings should be regarded as fundamental variables, from which all other data (including the root densities and correlation functions) can be derived. It was shown in [16] that the mean values of local charges only depend on the hole density of the 1-strings, and here we argued that the correlators depend on all higher $\rho_{h,j}$. Therefore, a large family of new root configurations with different correlations but the same local charges can be produced by artificially changing the higher hole densities in an arbitrary way. We presented an example for this procedure, with the numerical results shown in figure 1.

doi:10.1088/1742-5468/2014/09/P09026
In section 4.2 we calculated the GGE predictions for the quench from the dimer state using the TBA method. Our numerical data agree with those obtained in [19] using the QTM method. This agreement supports the validity of both approaches.

As an interesting by-product of our calculations, we found that the QA evaluated at the GGE saddle point solution is infinite. As a result, the spectral weight of the GGE solution (and in fact of all states with thermal asymptotics) decays faster than exponential as a function of the volume. In simple terms this means that the GGE solution is very far from the states selected by the QA, which actually determine the dynamics of the system.

Throughout this work the expression GGE was used in the conventional sense, meaning that the generalized statistical ensemble includes the local charges that are obtained by taking derivatives of the usual transfer matrix. New quasi-local operators have been found recently for the regime $\Delta < 1$ [36–38] and it is an interesting open question whether the addition of these new operators to the GGE is enough to fix all hole densities to their correct values, thus making the GGE complete and correct. Unfortunately the construction of [36–38] does not produce local operators for $\Delta > 1$, and it remains to be seen whether new charges can be produced by other means in this regime.

Acknowledgments

We are grateful to Gábor Takács and Márton Kormos for many useful discussions, which inspired the present work. Also, we are thankful to Márton Mestyán for his suggestion for evaluating the QA at the GGE-TBA saddle point solution. We are also grateful to Jean-Sébastien Caux and Jacopo De Nardis for useful discussions and for sending examples of their numerical data to us. We would like to thank Márton Kormos for valuable suggestions on the manuscript.

Appendix A. Correlation functions

In this section we show how to compute local correlators in the XXZ spin chain using the functions $\rho_{h,k}(\lambda)$, which are the densities of holes for the $k$-strings. As a first step one computes the root densities $\rho_{h,k}(\lambda)$ from (19) and the functions $\eta_k(\lambda) = \rho_{h,k}(\lambda)/\rho_{r,k}(\lambda)$. The $\eta_k$ are then used as the input to further linear equations.

Let us define

$$d^{(a)}(u) = \left(\frac{\partial}{\partial u}\right)^a d(u) \quad \quad \tilde{d}^{(a)}(u) = \left(\frac{\partial}{\partial u}\right)^a \tilde{d}(u), \quad \quad (A.1)$$

where $d(u)$ is given by (20) and

$$\tilde{d}(u) = -\sum_{n=1}^{\infty} \sin(2nu) \frac{\sinh(\eta_n)}{\cosh^2(\eta_n)} \quad \quad (A.2)$$

These functions satisfy the relations

$$\frac{\partial}{\partial \eta} d^{(a)}(u) = \frac{\partial}{\partial u} \tilde{d}^{(a)}(u). \quad \quad (A.3)$$
Let us introduce auxiliary functions $\rho^{(a)}_k$ and $\sigma^{(a)}_k$ that satisfy
\[
\rho^{(a)}_k(u) = \delta_{k,1} d^{(a)}(u) + d \cdot \left( \frac{\rho^{(a)}_{k-1}}{1 + 1/\eta_{k-1}} + \frac{\rho^{(a)}_{k+1}}{1 + 1/\eta_{k+1}} \right)
\]
\[
\sigma^{(a)}_k(u) = -\delta_{k,1} \tilde{d}^{(a)}(u) - d \cdot \left( \frac{\sigma^{(a)}_{k-1}}{1 + 1/\eta_{k-1}} + \frac{\sigma^{(a)}_{k+1}}{1 + 1/\eta_{k+1}} \right).
\] (A.4)

Note that the equation for $\rho^{(0)}_k$ coincides with (19), therefore it can be identified as $\rho^{(0)}_k = \rho_{a,k} + \rho_{b,k}$.

Using the notation
\[
f \cdot g = \int_{\pi/2}^{\pi/2} \frac{du}{2\pi} f(u)g(u)
\] (A.5)
we define the quantities
\[
\Omega_{a,b} = -2(-1)^{(j+k)/2} \left( (-1)^a G_{a+b} + d^{(b)} \cdot \frac{\rho_1^{(a)}}{1 + 1/\eta} \right) \] (A.6)
\[
\Gamma_{a,b} = 2(-1)^{(a+b-1)/2} \left( (-1)^b \tilde{G}_{a+b} + \tilde{d}^{(b)} \cdot \frac{\rho_1^{(a)}}{1 + 1/\eta} + d_1^{(b)} \cdot \frac{\sigma_1^{(a)}}{1 + 1/\eta} \right),
\]
where
\[
G_a = -2 \sum_{n=-\infty}^{\infty} \frac{(2ni)^a}{1 + e^{2\eta|n|}} \quad \tilde{G}_a = - \sum_{n=-\infty}^{\infty} \frac{|n|(2ni)^{a-1}}{\cosh^2(n\eta)}. \] (A.7)

The following symmetry properties hold:
\[
\Omega_{a,b} = \Omega_{b,a} \quad \Gamma_{a,b} = -\Gamma_{b,a}.
\]

Furthermore, $\Omega_{a,b}$ is non-vanishing if $a + b = 0 \mod 2$, whereas $\Gamma_{a,b}$ is non-vanishing if $a + b = 1 \mod 2$.

It can be shown that the auxiliary functions and the quantities $\Omega_{a,b}$ and $\Gamma_{a,b}$ are identical to those defined in [24]. The advantage of the above formulas over those of [24] is that here only neighbouring equations are coupled and $\Omega_{a,b}$ and $\Gamma_{a,b}$ are expressed using a single integral. This makes the numerical evaluation much more effective.

The numbers $\omega_{a,b}$ and $W_{a,b}$ are computed using
\[
\omega_{a,b} = -(-1)^{(a+b)/2} \Omega_{a,b} - (-1)^b \frac{1}{2} \left( \frac{\partial}{\partial u} \right)^{a+b} K(u) \bigg|_{u=0} \] (A.8)
\[
W_{a,b} = -(-1)^{(a+b-1)/2} \Gamma_{a,b} + (-1)^b \frac{1}{2} \left( \frac{\partial}{\partial u} \right)^{a+b} \tilde{K}(u) \bigg|_{u=0},
\]
where
\[
K(u) = \frac{\sinh 2\eta}{\sinh(u + \eta) \sinh(u - \eta)} \quad \tilde{K}(u) = \frac{\sinh(2u)}{\sinh(u + \eta) \sinh(u - \eta)}.
\]
Finally, local correlators are obtained by substituting $\omega_{a,b}$ and $W_{a,b}$ into the already available formulas of the QTM literature. Examples of such formulas can be found in [39]. The results for the nearest neighbour and next-to-nearest neighbour $z$–$z$ correlators are

$$
\langle \sigma^z_{1} \sigma^z_{2} \rangle = \coth(\eta)\omega_{0,0} + W_{1,0}
$$

(A.9)

$$
\langle \sigma^z_{1} \sigma^z_{3} \rangle = 2 \coth(2\eta)\omega_{0,0} + W_{1,0} + \tanh(\eta)\frac{\omega_{2,0} - 2\omega_{1,1}}{4} - \frac{\sinh^2(\eta)}{4}W_{2,1}.
$$

It follows from the original definitions in [24] that the numbers $\Omega_{a,0}$ are proportional to the local charges $\langle Q_a \rangle$. Constructing the generating function $G(\lambda)$ defined in (22) the formula (23) is easily derived from (A.6).

Appendix B. Numerical solution of the TBA equations with thermal asymptote

Here we describe a simple method to truncate the infinite system (37), which produces very accurate numerical data with a low number of equations. The basic idea is to use the exact asymptotes given by (39) and (41) by fixing the parameters $a$ and $\alpha$ at each iteration from one of the lower equations and substituting them into the final equation.

If the infinite set is truncated to $N_t$ equations, then the iterations are performed in the usual way for $j = 1, \ldots, N_t - 1$ and for the last equation we use

$$
\log \eta_{N_t} = d \times \log(1 + \eta_{N_t-1}) + \log(N_t + a + 1),
$$

(B.1)

where $a$ is extracted from the average of one of the other pseudo-energies:

$$
a = \sqrt{\left( \int \frac{du}{\pi} \eta_{N_t-b}(u) \right) + 1 + b - N_t}.
$$

(B.2)

We can choose for example $b = 2$. Concerning the iterations for $\rho_j$ we use

$$
\rho_{N_t} = d \times \frac{\rho_{N_t-1}}{1 + 1/\eta_{N_t-1}} + \frac{\alpha}{2(N_t + 1 + a)},
$$

(B.3)

where the parameter $\alpha$ can be fixed from one of the earlier equations similar to (B.2). The linear equations for the auxiliary functions $\rho_k^{(a)}$ and $\sigma_k^{(a)}$ needed for the correlation functions (see appendix A) can be iterated using (B.3) as well.

We observed that with this method, correlation functions can be obtained up to a precision of at least $10^{-11}$ with a small number of equations. For example at $\Delta = 2$ it was enough to choose $N_t = 10$, whereas for $\Delta = 1.4$ we chose $N_t = 14$. It was checked in all cases that the results for the correlators do not change as we vary $N_t$ or $b$, or the resolution of the rapidity axis for the integrations.

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