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The quench action approach to out-of-equilibrium quantum integrable models

Wouters, B.M.

Publication date
2015

Document Version
Final published version

Link to publication

Citation for published version (APA):
Wouters, B. M. (2015). *The quench action approach to out-of-equilibrium quantum integrable models*.

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Conclusions, overview and outlook

In this thesis we presented an extensive analysis of the quench action approach to out-of-equilibrium phenomena in quantum integrable models. We derived the quench action approach from first principles and saw applications to interaction quenches in the Lieb-Liniger model and the spin-1/2 XXZ chain. We also used the QA method to model the Bragg pulse on hard-core bosons. The most prominent results were as follows. First, we have established the broad applicability of the QA approach to quantum quench problems in integrable models. This mainly depends on the availability of overlaps and of their scaling towards the thermodynamic limit. Considering the universal features of the overlaps presented in this thesis and the recent derivation of recursive formulas for overlaps [174], there is good hope that other quenches can be studied by means of the QA approach in the near future.

Second, we found a failure of the GGE based on known local charges for the Néel-to-XXZ quench. Even the simplest nearest-neighbor correlators are predicted wrongly by the GGE and depending on the initial state [56, 57] the error can become of order one. A deeper understanding is still lacking, but will likely give a better understanding of the physics of relaxation in quantum integrable systems.

Third, we have seen a separation of relaxation timescales in the quantum Newton's cradle for the Tonks-Girardeau gas. After a Bragg pulse there is a short phase of rapid relaxation towards a temporary steady state governed by the GGE, followed by the oscillation in the trap at much longer timescales. Extensions of our methods to longer pulses and finite c could provide insights in the underlying physics of the absence of thermalization in the cradle experiment [24].

In the remainder of this chapter we briefly review other applications of the QA approach and present some preliminary steps towards new research directions inspired by the findings in this thesis.

7.1 Other applications of the QA approach

For the sake of completeness, we here give a very brief overview of other known applications of the QA approach. We permit ourselves to only state the results and for technical details we refer to the publications themselves. We repeat that in Refs [56, 57] the quench action logic was applied to the spin-1/2 XXZ chain in the gapped regime, with initial states the dimer and q-dimer state. Both method and conclusions, also regarding the failure of the GGE, were in agreement with the results discussed in this thesis for the Néel-to-XXZ quench.

Time evolution in the sine-Gordon model

In Ref. [58] a hybrid combination of GGE and QA logic is applied to specific quenches in the sine-Gordon model, which is a 1D integrable quantum field theory with Hamiltonian

$$\hat{H} = \frac{v}{16\pi}\int dx \left[(\partial_x\hat{\Phi})^2 + \frac{1}{v^2}(\partial_t\hat{\Phi})^2\right] - \lambda\int dx \cos(\beta\hat{\Phi})\,, \tag{7.1}$$

where $\hat{\Phi}(x,t)$ is a real, bosonic field. This model emerges as the low-energy limit of several 1D spins chains and systems of ultra-cold atoms. A very special class of initial states compatible with integrability is considered; coherent-like states with coefficients related to the scattering phase shift of the model. This makes it possible to obtain the overlaps with postquench Hamiltonian eigenstates.

First, in the repulsive regime $1/\sqrt{2} \leq \beta < 1$ the root density of the stationary state is computed by means of the local conserved charges. Note that this approach is inspired by the GGE logic and unlike the QA method, where overlaps are used directly to derive GTBA equations. The root density is used in the quench action result Eq. (3.20) to obtain the time evolution at late times for the local observable $e^{i\beta\hat{\Phi}(x,t)/2}$. The final result (only valid for low densities of excitations of the postquench Hamiltonian) is an exponential decay $\langle\psi_0|e^{i\beta\hat{\Phi}(x,t)/2}|\psi_0\rangle = a_0\, e^{-b_0 t} + \ldots$, with both coefficients a_0, b_0 known analytically. This is confirmed with an independent linked-cluster computation.

This constitutes the first example of an analytical computation of the time evolution of a local observable after a quench to a truly interacting integrable model. It should be noted that this result is only valid in a very restrictive setting. In particular, generalizing to other observables might be difficult and it is not at all clear how these very specific initial states can be realized in actual experiments.

Geometric quench for free fermionic chain

In Ref. [59] a geometric quench to the spin-1/2 XX chain (the XXZ chain with anisotropy $\Delta = 0$) is considered. Two half-infinite chains, both in a thermal state at different temperatures, are joined at a certain time such that translational invariance is restored. This quench protocol had been studied before (see e.g. Refs [217, 218]) and two late-time regimes were observed. For late times much smaller than L/v_{max}, where L is system size and v_{max} is the velocity of the fastest mode in the system, a nonequilibrium steady state with two energy currents arises. For much longer times boundary effects start playing a role. The energy currents phase out and time-reversal symmetry is restored.

The spin-1/2 XX chain is equivalent to free fermions. This can be used to write the overlaps between pre- and postquench eigenstates as determinants of matrix elements of single-particle operators, as is done in Ref. [59]. Contrary to the quenches studied in this thesis the initial state is a mixed state, characterized by two temperatures. This can be used to factorize and exponentiate the overlaps, after which a quench action S_{QA} is obtained. A saddle-point approximation and a careful handling of the order of limits reproduces the momentum distribution of both late-time regimes. This application of the QA approach to geometric quenches might be extended in the future to truly interacting systems such as the Lieb-Liniger model, as the authors suggest.

Driving terms for the Kondo model

In Ref. [60] the driving terms of the GTBA equations for the (isotropic) Kondo model are derived. The model represents a single spin-1/2 impurity coupled to the local spin density of a bath of noninteracting electrons,

$$\hat{H} = \int dx \Big[- i\hat{\psi}^{\dagger}_{\sigma}(x)\partial_x\hat{\psi}_{\sigma}(x) + \tfrac{I}{2}\hat{\psi}^{\dagger}_{\sigma}(0)\vec{\sigma}_{\sigma\sigma'}\hat{\psi}_{\sigma'}(0)\cdot\vec{S}\Big] , \tag{7.2}$$

where summation over repeated indices is implicit. A state of free electrons without impurity is considered as initial state and the observable of interest is the Loschmidt echo, which gives a time-dependent contribution to the driving terms.

The coordinate Bethe Ansatz for the Kondo model distinguishes between spin and charge degrees of freedom of the electrons. As a consequence, the Bethe equations are nested and the overlaps with the initial state can be decomposed in a part for spin and a part for charge. The difficult part concerns the spin, whose overlaps are given in terms of determinants by Slavnov's formula [110]. To treat these expressions in the thermodynamic limit, the variation of the determinant with respect to the root densities (i.e. the driving term) is expressed in terms of coupled linear integral equations. A possible application to experimentally observable quantities is the current at intermediate voltages [219].

7.2 Open problems and outlook

7.2.1 Towards modifying the GGE

We have seen different instances of quantum quenches to truly interacting systems where the GGE based on local conserved charges (given by the algebraic Bethe Ansatz) failed to reproduce the postquench steady state. Nonetheless, the intuitive notion from statistical physics that equilibrium values of local operators can be described by a relatively small number of parameters is still alluring. As discussed, several promising attempts to modify the notion of a GGE are underway [202, 203, 204, 205, 168]. What these pursuits have in common is that they try to increase the set of charges that determines the GGE and thereby increase the number of constraints on the steady state.

Here we present preliminary results of a different approach, where we try to construct a density matrix for the BEC-to-LL quench directly from the overlaps and the QA logic. The reason for this is twofold. The form of the density matrix might shed light on the finite (local) conserved charges that play a role in the postquench equilibrium. Secondly, its form could tell us something about a general theory of quantum quenches applicable to a larger set of initial states. We will express the density matrix as an infinite product of the transfer matrices evaluated at different values of the spectral parameter. We stress that it is natural to advance in this way, as the transfer matrix comprises all conserved charges of the theory and the logic of the GGE is that a subset of these charges determines the statistical ensemble.

The idea of writing the statistical operator as a product of transfer matrices is a crucial step in the quantum transfer matrix approach [20, 21, 22, 23] in order to obtain integral formulas for thermodynamic quantities and local correlation functions at finite temperature. Using the Trotter-Suzuki mapping, one can show for the XXZ chain that in the thermodynamic limit a specific product of transfer matrices converges to the thermal density matrix [20, 16]. In Ref. [126] this was generalized to the truncated GGE.

The density matrix is an operator that encodes the different weights of states in the statistical ensemble corresponding to the postquench equilibrium. Given a quench from an initial state $|\psi_0\rangle = |\mathrm{BEC}\rangle$, we define a finite-size operator $\hat{\varrho}_{\psi_0}$ such that for any local operator $\hat{\mathcal{O}}$ the equilibrium is determined by

$$\langle \rho^{\mathrm{sp}}|\hat{\mathcal{O}}|\rho^{\mathrm{sp}}\rangle = \lim\nolimits_{\mathrm{th}} \frac{\mathrm{Tr}_{\mathcal{H}}\left[\hat{\varrho}_{\psi_0}\hat{\mathcal{O}}\right]}{\mathrm{Tr}_{\mathcal{H}}\left[\hat{\varrho}_{\psi_0}\right]} = \lim\nolimits_{\mathrm{th}} \frac{\sum_{\boldsymbol{\lambda}} \varrho_{\psi_0}(\boldsymbol{\lambda})\langle\boldsymbol{\lambda}|\hat{\mathcal{O}}|\boldsymbol{\lambda}\rangle}{\sum_{\boldsymbol{\lambda}} \varrho_{\psi_0}(\boldsymbol{\lambda})} , \tag{7.3}$$

where ρ^{sp} is the saddle-point root density given in Eqs (4.25) and $\varrho_{\psi_0}(\boldsymbol{\lambda}) = \langle\boldsymbol{\lambda}|\hat{\varrho}_{\psi_0}|\boldsymbol{\lambda}\rangle$. We work with this finite-size formulation of the density matrix for technical convenience. In the end, only in the thermodynamic limit the notions of a density matrix and statistical ensemble make sense. The reader should keep this in mind. Also observe that we assumed that the finite-size density matrix commutes with the Hamiltonian.

The eigenvalues of the transfer matrix $\hat{\tau}$ of the Lieb-Liniger model were given in Eq. (2.74). Let us denote the eigenvalues on a parity-invariant Bethe state $|\tilde{\boldsymbol{\lambda}}\rangle$ in the following way: $\tau(\mu, \tilde{\boldsymbol{\lambda}}) = \tau_+(\mu, \tilde{\boldsymbol{\lambda}}) + \tau_-(\mu, \tilde{\boldsymbol{\lambda}})$, with

$$\tau_\pm(\mu, \tilde{\boldsymbol{\lambda}}) = \exp\left(\mp\frac{i\mu L}{2}\right)\prod_{j=1}^{N/2} \frac{(\mu \pm ic)^2 - \lambda_j^2}{\mu^2 - \lambda_j^2} . \tag{7.4}$$

Observe that $\tau_+(\mu, \tilde{\boldsymbol{\lambda}}) = \tau_-(-\mu, \tilde{\boldsymbol{\lambda}})$. Given a positive integer $w \geq 1$ and a finite-size Bethe state $|\tilde{\boldsymbol{\lambda}}\rangle$, let us define a new (real and nonnegative) quantity,

$$\Theta_{\psi_0}(w, \tilde{\boldsymbol{\lambda}}) = \frac{1}{w^{2N}} \prod_{m=0}^{w} e^{-\frac{mcL}{4}} \tau_+(imc/2, \tilde{\boldsymbol{\lambda}}) = \frac{1}{\prod_{j=1}^{N/2} \frac{\lambda_j^2}{c^2}\left(\frac{\lambda_j^2}{c^2} + \frac{1}{4}\right)} + O\left(\frac{\lambda_j}{cw}\right), \tag{7.5}$$

where the second equality follows from elementary manipulations and the first term in the last line can be recognized as part of the overlaps squared for the BEC-to-LL quench, given in Eq. (4.3a). It is this part that determined the quench action saddle point in Chapter 4. We therefore conclude that

$$\langle \rho^{\rm sp}|\hat{\mathcal{O}}|\rho^{\rm sp}\rangle = \lim_{w\to\infty} \lim\nolimits_{\rm th} \frac{\sum_{\tilde{\boldsymbol{\lambda}}} \Theta_{\psi_0}(w, \tilde{\boldsymbol{\lambda}}) \langle \tilde{\boldsymbol{\lambda}}|\hat{\mathcal{O}}|\tilde{\boldsymbol{\lambda}}\rangle}{\sum_{\tilde{\boldsymbol{\lambda}}} \Theta_{\psi_0}(w, \tilde{\boldsymbol{\lambda}})}\,. \tag{7.6}$$

It is important to understand the limit $w \to \infty$ correctly. The thermodynamic limit is taken before the cutoff w is sent to infinity, and consequently the saddle-point equation and its solution depend on the finite parameter w. It is easy to see that this dependence disappears in the limit $w \to \infty$ and that the solution to the saddle-point equation converges to $\rho^{\rm sp}$. At finite, large w the GTBA equation only gets deformed for rapidities $\lambda > wc$ and this deformation can be pushed to infinity.

The quantity $\Theta_{\psi_0}(w, \tilde{\boldsymbol{\lambda}})$ is a product of $\tau_+(\mu, \tilde{\boldsymbol{\lambda}})$ evaluated at different values of the spectral parameter on the imaginary axis. Unlike for $\tau(\mu, \tilde{\boldsymbol{\lambda}})$, there is no known corresponding operator $\hat{\tau}_+(\mu)$ whose eigenvalues on parity-invariant Bethe states are given by $\tau_+(\mu, \tilde{\boldsymbol{\lambda}})$. However, we claim that the density matrix in Eq. (7.3) for the BEC-to-LL quench is given by

$$\hat{\varrho}_{\psi_0} = \prod_{m=0}^{\infty} \hat{\tau}(imc/2)\,, \tag{7.7}$$

where the product consists of the transfer matrix evaluated on all (half)integer points on the positive imaginary axis, including the origin. Before discussing the evidence for this claim, a couple of remarks are in order. First, the overall constant factors of $\Theta_{\psi_0}(w, \tilde{\boldsymbol{\lambda}})$ were left out because they do not affect the saddle point and they cancel between numerator and denominator in Eq. (7.3). Second, the infinite product should be understood as a product with a large cutoff that is sent to infinity after the thermodynamic limit in Eq. (7.3) has been taken. This is analogous to the order of limits in Eq. (7.6). Third, the sums over the Hilbert space in Eq. (7.3) must be restricted to parity-invariant Bethe states. This is not a very restrictive limitation and does not make our claim trivial. Out of all parity-invariant states the density matrix defined in Eq. (7.7) precisely isolates the correct saddle-point state of the BEC quench.

Now, we will argue why the conjectured density matrix in Eq. (7.7) leads to the right-hand side of Eq. (7.6). To show this we have to prove that in traces over the density matrix, in the thermodynamic limit, only the τ_+ part of the eigenvalues survives and the τ_- can be neglected. To see this, assume Eq. (7.7) and observe that for fixed cutoff w, restricted to parity-invariant states and up to an irrelevant overall factor, the elements of the density matrix in Eq. (7.3) are given by

$$\begin{aligned} &\langle \tilde{\boldsymbol{\lambda}} | \hat{\varrho}_{\psi_0} | \tilde{\boldsymbol{\lambda}} \rangle \qquad (7.8) \\ &\sim \tau(0, \tilde{\boldsymbol{\lambda}}) \prod_{m=1}^{w} \left[\prod_{j=1}^{N/2} \frac{(m/2+1)^2 c^2 + \lambda_j^2}{m^2 c^2/4 + \lambda_j^2} + e^{-\frac{mcL}{2}} \prod_{j=1}^{N/2} \frac{(m/2-1)^2 c^2 + \lambda_j^2}{m^2 c^2/4 + \lambda_j^2} \right], \end{aligned}$$

where we used that $\tau_+(0, \tilde{\boldsymbol{\lambda}}) = \tau_-(0, \tilde{\boldsymbol{\lambda}})$. Expanding this products gives 2^w terms, and each term leads to a different saddle point when the thermodynamic limit of the sums over the Hilbert space in Eq. (7.3) is taken. Each of these terms is identified with a vector $\vec{p}$ of length w and with components either $+1$ or -1. A $+1$ on position m means a choice for the τ_+ part in the mth factor of the product, and likewise a -1 for the τ_- part. The term identified with vector $\vec{p}$ has in the thermodynamic limit an extensive exponential part given by $-S_{(w,\vec{p})}$, with

$$S_{(w,\vec{p})}[\rho] = L \int_0^\infty d\lambda \Big(\rho(\lambda)\, g_{(w,\vec{p})}(\lambda) - s_{\mathrm{YY}}[\rho, \lambda] \Big) + \frac{cL}{4} \sum_{m=1}^{w} (1 - p_m)\, m\,, \quad (7.9a)$$

where the Yang-Yang entropy density $s_{\mathrm{YY}}[\rho, \lambda]$ was defined in Eq. (2.42e) and p_m is the mth component of $\vec{p}$. The driving term $g_{(w,\vec{p})}$ is given by

$$g_{(w,\vec{p})}(\lambda) = -\log \left[\frac{\lambda^2 + c^2}{\lambda^2} \prod_{m=1}^{w} \frac{(m/2 + p_m)^2 c^2 + \lambda^2}{m^2 c^2/4 + \lambda^2} \right]. \quad (7.9b)$$

Note that $S_{(w,\vec{p})}$ is the equivalent of the quench action S_{QA} of a quantum quench. And for the specific case $\vec{p} = (1, 1, \dots, 1)$ the quantity $\lim_{w\to\infty} \big(S_{(w,\vec{p})} + 4\log(w) \big)$ is precisely the quench action for the BEC-to-LL quench. For each vector $\vec{p}$ and associated action $S_{(w,\vec{p})}$ a saddle-point approximation can be performed, which is exact in the thermodynamic limit. The resulting GTBA equation is like Eq. (4.16a), but with the driving term replaced by $g_{(w,\vec{p})}$, leading to a saddle-point density denoted by $\rho_{(w,\vec{p})}$. We claim that for any $w \geq 1$, the term with $\vec{p} = (1, 1, \dots, 1)$ has the dominant saddle point and all other terms are exponentially suppressed, i.e.

$$S_{(w,\vec{p})}[\rho_{(w,\vec{p})}] > S_{(w,(1,1,\dots,1))}[\rho_{(w,(1,1,\dots,1))}]\,, \quad (7.10)$$

for any vector $\vec{p}$ that is not given by $(1, 1, \dots, 1)$. For small values of w, we have solved the GTBA equations and computed the action $S_{(w,\vec{p})}$ on the saddle point.

The results are in agreement with our claim, as can be seen in Fig. 7.1. Broadly speaking, replacing more $+1$'s by -1's in the vector $\vec{p}$ leads to a larger on-shell action $S_{(w,\vec{p})}[\rho_{(w,\vec{p})}]$. We have numerically verified the inequality for all vectors $\vec{p}$ with at most two minuses up to $w = 100$. This is not a full-fledged proof, but there is no reason to suspect that for large w the inequality in Eq. (7.10) might fail. We therefore conclude that in the thermodynamic limit the term with only τ_+ factors is dominant and all other terms are exponentially suppressed. This proves that the density matrix in Eq. (7.7) leads to the right-hand side of Eq. (7.6). As an example, in Fig. 7.1 the convergence for increasing w towards the exact saddle-point density of the BEC-to-LL quench is displayed.

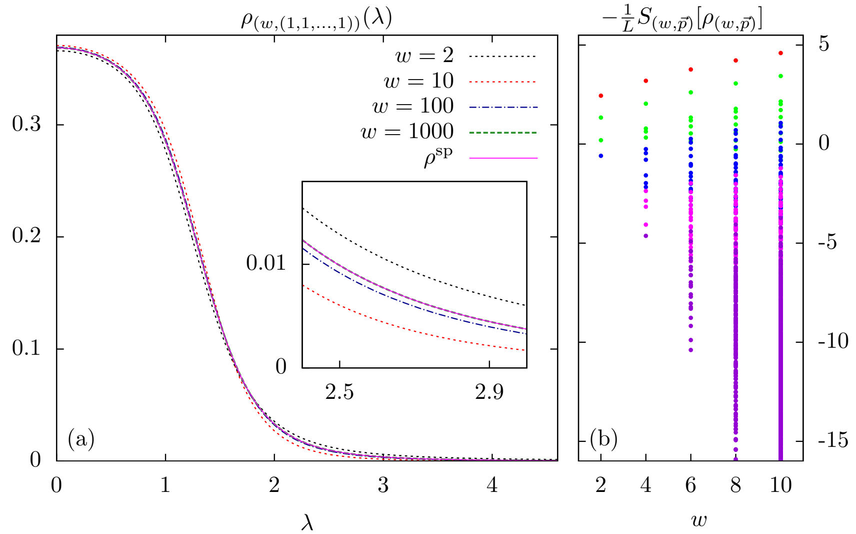

Figure 7.1: (a) Saddle-point densities $\rho_{(w,(1,1,\ldots,1))}$ for increasing w are compared with the exact saddle-point density of the BEC-to-LL quench [see Eqs (4.25)]. To obtain normalizable densities at finite w one must include a regulator in the GTBA driving term. This regulator is a consequence of the correction term in Eq. (7.5) and is negligible when $\lambda \ll cw$. For large w the specific form of the regulator becomes unimportant. *Inset:* Zoom. (b) The on-shell exponents $-\frac{1}{L}S_{(w,\vec{p})}[\rho_{(w,\vec{p})}]$ for all possible vectors $\vec{p}$ for $w = 2, 4, 6, 8, 10$. The color scheme signifies the total number of minuses in $\vec{p}$: zero (red), one (green), two (blue), three (pink) or more than three (purple). All computations were performed for $c = n = 1$.

We have thus found a form of the statistical density operator in terms of the transfer matrix that reproduces the saddle point after a BEC-to-LL quench. It is an infinite product of transfer matrices with spectral parameters evaluated on all (half)integer points on the positive imaginary axis, including the origin. It is tempting to write the density matrix in a GGE-like form [see Eqs (3.6)],

$$\hat{\varrho}_{\text{BEC}} = \exp\left(\sum_{m=0}^{\infty} \log[\hat{\tau}(imc/2)]\right) . \tag{7.11}$$

However, the operators in the sum are all highly nonlocal. As we have seen in Chapter 2, the local conserved charges are obtained from an expansion of $\log[\hat{\tau}(\mu)]$ around $\mu = i\infty$. The relation between this form of the density matrix and the GGE is an interesting open problem apt for future research and might give hints for an improved formulation of the GGE with finite local charges in the BEC-to-LL quench.

Even more interesting would be an extension of the above analysis to the Néel quenches in the spin-1/2 XXZ chain. Since the GGE based on all known local charges fails, an operator form of the density matrix could shed light on the question which other charges, possibly nonlocal, must be included to correctly reproduce the postquench saddle point. Unfortunately, there are several complications. It turns out that the transfer matrix for XXZ is a nonsmooth operator, rendering the QA logic inapplicable. Furthermore, replacing $\tau_+(\mu, \tilde{\boldsymbol{\lambda}})$ by $\tau_+(\mu, \tilde{\boldsymbol{\lambda}}) + \tau_-(\mu, \tilde{\boldsymbol{\lambda}})$ is not allowed for the inverse of the transfer matrix, which one encounters for the Néel-to-XXZ quench. For details on this attempt and the first example of a nonsmooth operator, see Appendix E.

7.2.2 Quenches to the gapless spin chain

In Section 5 we quenched the zero-momentum Néel state to the gapped regime of the XXZ spin chain. It is an open question how this extends to the gapless regime $-1 < \Delta < 1$. This is interesting because quenches across quantum critical points could exhibit dynamical phase transitions, where the time dependence of the Loschmidt echo is nonanalytic at a certain critical time [140]. The QA approach is in principle able to reproduce the time evolution for the spin-1/2 XXZ chain and can be used as a vehicle to study these phenomena.

In Appendix F the GTBA equations for the Néel-to-XXZ quench to the gapless regime can be found, as well as the GGE integral equations and $\rho_{1,h}$. A peculiar feature of the gapless regime is that for rational values of $\gamma = \arccos(\Delta)$ only a finite number of string types is allowed. The GTBA equations form a finite set of coupled integral equations and when numerically evaluated there is no need for a truncation.

Numerical analysis shows that the GTBA equations for the GGE can be solved consistently and the resulting correlators at the GGE saddle point change continuously through the XXX point from the gapped to the gapless regime. However, the quench action GTBA equations (F.10), combined with the BGT equations (F.7) do not produce a correctly normalized set of root densities. There is no chemical potential such that all densities add up to half filling, even for very simple values of γ where only a few string types are allowed. It is clear that not everything is understood for this type of quenches and further research is required.

7.2.3 Other topics for future research

Throughout the thesis many ideas for future research were already presented. Here we ennumerate the most pressing questions according to the author. Applying the QA approach to other quantum quenches could lead to a more general understanding of out-of-equilibrium dynamics in integrable models. For example, it would be very interesting to generalize the Néel overlaps to overlaps for generic product states or to study geometric quenches in truly interacting models. Ultimately we would like to be able to solve very general quench problems, for example from c' to c in the Lieb-Liniger model and from Δ' to Δ in the spin chain. This however is still far away from what we can do at this moment.

Second, the failure of the GGE in the spin-1/2 XXZ chain begs for a better understanding. Whether and how more (quasi-)local charges could repair the GGE is a very interesting open problem. The standard formulation of the GGE does not specify which conservation laws are important in the description of the postquench equilibrium. Developing an intuition for this, maybe in terms of a classification of charges, would be a huge step forward.

Although most of this thesis focused on the equilibrium at late times after a global quantum quench, the QA approach also purports to give the postquench time evolution in the thermodynamic limit for any time after the quench. Progress on this was made in Refs [58, 54, 55], but a more extensive implementation is desirable. In particular, time evolution for the Néel-to-XXZ quench is an interesting open problem. A first step in this direction requires the nearly diagonal matrix elements of simple operators in the thermodynamic limit.