The dynamical free energy and the Loschmidt echo for a class of quantum quenches in the Heisenberg spin chain

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Abstract. We consider a class of global quantum quenches in the Heisenberg XXZ spin chain, where the initial states are given by products of local two-site states. The two main examples are the Néel state and the dimer state. We derive an exact analytic result for the ‘Loschmidt echo per site’ at imaginary times and also consider the analytic continuation back to real times. As a by-product we obtain an exact result for the ‘overlap per site’ between the Néel state and the ground state of the XXZ Hamiltonian in the massive regime.

Keywords: integrable spin chains (vertex models), quantum integrability (Bethe ansatz), exact results

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### 1. Introduction

The non-equilibrium dynamics of quantum systems, in particular quantum quenches, have attracted a lot of interest lately. One of the main questions is whether an isolated quantum system equilibrates, and, if so, what the stationary values of physical observables are and how they depend on the initial state and the Hamiltonian governing the time evolution. Generally one expects thermalization, which means that the stationary values of observables coincide with those calculated from a thermal ensemble with a given temperature [1].

Integrable models provide an interesting setting where the real-time dynamics can be markedly different. These theories possess higher conserved charges, which prevent thermalization in the usual sense. Instead, it was proposed in [2] that in the long-time limit the mean values of observables are given by the so-called generalized Gibbs ensemble (GGE), which incorporates all conserved charges with appropriate Lagrange-multiplers.

Most previous work has focused on integrable spin chains which are equivalent to free fermions [3]–[14] or models which can be treated by conformal field theory methods [15]. Considerable work has been undertaken to understand the quench dynamics of the 1D Bose gas, especially in the infinite interaction limit [16]–[18]. Concerning interacting theories
not equivalent to free fermions there are only a few analytic results available \cite{19, 20} and even the numerical treatment based on the Bethe Ansatz solution is challenging \cite{21}.

The Heisenberg spin chain is a paradigmatic integrable model, which is one of the simplest genuinely interacting models. However, the questions of equilibration and thermalization are very far from being solved. The first two papers to consider the GGE for the XXZ spin chain were \cite{23} and \cite{24}. Both developed the so-called quantum transfer matrix formalism for the GGE and gave approximate predictions for the long-time limit of local correlators following a quench from the Néel state. In \cite{23} a truncated GGE was used, whereas \cite{24} took into account all higher charges in a $1/\Delta$ expansion. We would like to stress that both papers bypass the derivation of the actual time dependence and assume the GGE hypothesis to provide predictions which could be checked by other methods.

One of the reasons for the lack of rigorous results for non-equilibrium dynamics in the XXZ spin chain is that the celebrated Bethe Ansatz solution is only adequate for equilibrium problems. Calculation of the real-time dynamics requires one to take into account all states (or at least a large subset of them \cite{22}), which is a notoriously difficult task. Moreover, one needs manageable formulae for overlaps of Bethe states and the initial state, which are typically not available either.

Apart from the correlation functions there has been recent interest in the Loschmidt echo (the overlap of the initial and time-evolved states) too, which is a somewhat simpler quantity, yet it possesses unexpected features. In \cite{26, 27} it was observed that the Loschmidt echo displays non-analytic behaviour if the system is quenched across a critical point. This problem was considered in the very recent work \cite{25}, where Fagotti derived analytic results for the Loschmidt echo per site in the XXZ chain using the GGE hypothesis for the exponential of the Hamiltonian. The non-linear integral equations (NLIEs) of \cite{25} are implicit in the sense that Lagrange-multipliers are not specified; nevertheless it was shown that numerical results can be calculated in the $1/\Delta$ approximation and the analytic properties of functions involved in the NLIEs can be studied.

In this work we derive an exact analytic result for the Loschmidt echo per site for the case of purely imaginary times and we also consider the analytic continuation back to real times. To the best of our knowledge this is the first exact result concerning the time dependence of a physical quantity in a non-equilibrium setting of the interacting XXZ chain.

The structure of the paper is as follows. In section 2 we present the problem and the general notations. In section 3 we develop the Trotter–Suzuki decomposition for the Loschmidt echo at imaginary times and show that the problem is equivalent to finding the leading eigenvalue of the so-called boundary quantum transfer matrix (BQTM). In section 4 we diagonalize the BQTM using the already available techniques of the boundary algebraic Bethe Ansatz. In section 5 the resulting equations are worked out for a quench from the Néel state. Section 5.4 includes numerical results and our investigations on the analytic continuation to real times. Section 6 is devoted to the XXX limit and the quench starting from the dimer state. We conclude in section 7.

2. The dynamical free energy density and the Loschmidt echo

Consider a quantum quench situation in a 1D spin chain, where at $t = 0$ the system is prepared in a state $|\Psi_0\rangle$ and for $t > 0$ its time evolution is governed by a Hamiltonian of

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the form

\[ H = \sum_{j=1}^{L} u_j + h_{j,j+1}, \tag{2.1} \]

where \( u_j \) and \( h_{j,j+1} \) are one-site and two-site operators, \( L \) is the length of the chain and periodic boundary conditions are assumed. The state \( |\Psi_0\rangle \) can be chosen as the ground state of another local Hamiltonian \( H_0 \), or it can be prepared according to some well-defined rule. Specific examples for \( |\Psi_0\rangle \) will be given later.

In this work we focus on the cumulant generating function and the Loschmidt echo.

The cumulant generating function \( G(s) \) is defined as

\[ \exp G(s) = |\langle \Psi_0 | \exp(-sH) | \Psi_0 \rangle|, \quad s \in \mathbb{R}^+. \tag{2.2} \]

It satisfies the initial condition \( G(0) = 0 \) and its power series in \( s \) defines the cumulants of \( H \),

\[ G(s) = \sum_{n=1}^{\infty} \kappa_n \frac{s^n}{n!}. \tag{2.3} \]

The first few cumulants are

\[ \begin{align*}
\kappa_1 &= -\langle \Psi_0 | H | \Psi_0 \rangle \\
\kappa_2 &= \langle \Psi_0 | H^2 | \Psi_0 \rangle - \langle \Psi_0 | H | \Psi_0 \rangle^2 \\
\kappa_3 &= -\langle \Psi_0 | H^3 | \Psi_0 \rangle + 3\langle \Psi_0 | H^2 | \Psi_0 \rangle \langle \Psi_0 | H | \Psi_0 \rangle - 2\langle \Psi_0 | H | \Psi_0 \rangle^3.
\end{align*} \tag{2.4} \]

It is easy to see that every \( \kappa_n \) is linear in \( L \) once \( L > n \).

It is useful to introduce the function

\[ g(s) = \lim_{L \to \infty} \frac{G(s)}{L}. \tag{2.5} \]

Its power series expansion is given by

\[ g(s) = \sum_{n=1}^{\infty} \tilde{\kappa}_n \frac{s^n}{n!}, \tag{2.6} \]

with

\[ \tilde{\kappa}_n = \lim_{L \to \infty} \frac{\kappa_n}{L}. \]

Note that even though \( g(s) \) is well defined through (2.5), the expansion (2.6) is typically not a convergent series, as the \( L \to \infty \) limit is not uniformly convergent.

The function \( g(s) \) is the main object of interest of this work. It is analogous to the free energy density if \( s \) is interpreted as an inverse temperature. Following [25] we call it the dynamical free energy density.

The Loschmidt echo is defined as the overlap of the time-evolved state and the initial state,

\[ M(t) = |\langle \Psi_0 | \exp(-itH) | \Psi_0 \rangle|^2. \]
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For any finite $t$ it decays exponentially with the volume. Therefore it is useful to define the ‘Loschmidt echo per site’,

$$m(t) = M(t)^{1/L}.$$ 

It follows from the formulae above that the Loschmidt echo per site is given by the analytic continuation of the dynamical free energy density,

$$\log m(t) = 2\text{Re}(g(it)).$$

At any real $s$ the object in (2.2) is equivalent to a partition function of a 2D classical system with boundary conditions specified by the state $|\Psi_0\rangle$. This correspondence will be used below to derive exact analytic results for $g(s)$, $s \in \mathbb{R}^+$ for a class of quantum quenches in the XXZ Heisenberg spin chain. The analytic continuation to $s = it$ is considered in section 5.4.

### 3. The Hamiltonian, the initial states and the Trotter–Suzuki decomposition

The Hamiltonian of the XXZ Heisenberg spin chain is

$$H = \sum_{j=1}^{L} (\sigma^x_j \sigma^x_{j+1} + \sigma^y_j \sigma^y_{j+1} + \Delta(\sigma^z_j \sigma^z_{j+1} - 1)).$$ (3.1)

The anisotropy parameter $\Delta$ can be chosen arbitrarily; the $\Delta = 1$ case specifies the SU(2) symmetric XXX Hamiltonian.

We consider initial states $|\Psi_0\rangle$ which are constructed as products of two-site states,

$$|\Psi_0\rangle = |v\rangle \otimes |v\rangle \otimes \cdots \otimes |v\rangle.$$ (3.2)

Here $|v\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2$ is of the form

$$|v\rangle = \frac{1}{\sqrt{1 + |\gamma|^2}} (|+\rangle + \gamma |\rangle - +\rangle).$$ (3.3)

The following two particular cases will be considered.

- The case $\gamma = 0$ which is simply the Néel state $|N\rangle = |+\cdots +\rangle$. This state is one of the two ground states of the Hamiltonian in the $\Delta \to \infty$ limit.
- The case $\gamma = -1$ which we call the fully dimerized, or simply dimer state. This state is SU(2) symmetric and it is one of the two ground states of the Majumdar–Ghosh Hamiltonian [28]

$$H_{\text{MG}} = \sum_j \sigma_j \cdot \sigma_{j+1} + \frac{1}{2} \sum_j \sigma_j \cdot \sigma_{j+2}.$$ 

In both cases the other ground state is obtained by translation by one site.

#### 3.1. The Suzuki–Trotter decomposition

The expectation value in (2.2) can be computed using the Suzuki–Trotter decomposition

$$\exp(-sH) = \lim_{N \to \infty} \left(1 - \frac{sH}{N}\right)^N.$$ (3.4)
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\[
\begin{align*}
+ & \quad \sinh(u + \eta) \quad + \quad \sinh(u) \quad + \quad \sinh(\eta) \\
+ & \quad \sinh(u + \eta) \quad + \quad \sinh(u) \quad + \quad \sinh(\eta)
\end{align*}
\]

**Figure 1.** The six-vertex model weights as specified by the trigonometric \( R \)-matrix (3.7). Here \( u \) is attached to the horizontal line and 0 to the vertical one.

\[
\begin{array}{llllll}
\hline
\hline
j & & & & & k \\
\hline
\end{array}
\]

\[ T_{jk}(u) \]

**Figure 2.** The monodromy matrix of the periodic system of length \( L \). The horizontal line carries rapidity \( u \), whereas the inhomogeneities of the vertical lines are zero. The \( R \)-matrix acts on the vertices with matrix elements given by the six-vertex model weights depicted in figure 1.

In order to evaluate the \( N \)-fold product we use the algebraic Bethe Ansatz [29] and the quantum transfer matrix technique [30, 31]. As a first step we introduce the (rapidity dependent) monodromy matrix of the periodic spin chain as

\[
T(u) = L_L(u) \cdots L_1(u). \tag{3.5}
\]

Here \( L_j(u) \) are local Lax-operators given by

\[
L_j(u) = R_{0j}(u), \tag{3.6}
\]

where \( R(u) \) is the trigonometric \( R \)-matrix given by

\[
R(u) = \begin{pmatrix}
\sinh(u + \eta) & & \\
\sinh(u) & \sinh(\eta) & \\
\sinh(\eta) & \sinh(u) & \\
\sinh(u + \eta) & & \\
\end{pmatrix}, \tag{3.7}
\]

where the parameter \( \eta \) is related to the anisotropy by \( \Delta = \cosh \eta \). The index \( j \) in (3.6) refers to the site \( j \) of the spin chain, whereas 0 refers to the so-called auxiliary space. The monodromy matrix is represented pictorially in figure 2.

The transfer matrix is defined as the trace in auxiliary space

\[
t(u) = \text{Tr}_0 T(u). \tag{3.8}
\]

It is known that \( t(0) \) is proportional to the translation operator and the linear term in \( u \) generates the Hamiltonian [31]. In the present normalization the following relation holds for large \( N \):

\[
t(-\beta/2N)t(-\eta + \beta/2N) \frac{1}{(\sinh(-\beta/2N + \eta))^{2L}} = 1 - \frac{\beta}{N}Q_2 + \cdots,
\]

where

\[
Q_2 = \frac{1}{2\sinh(\eta)} H_{XXZ}.
\]

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Figure 3. The so-called quantum monodromy matrix, which acts on an auxiliary spin chain of length $2N$, where $N$ is the Trotter number. The inhomogeneities associated with the vertical lines are $a_1 = \beta/2N$ and $a_2 = -\beta/2N - \eta$.

Figure 4. The boundary transfer matrix with inhomogeneities $\xi_j$.

Therefore

$$
\langle \Psi_0 | \exp(-sH) | \Psi_0 \rangle = \lim_{N \to \infty} \frac{1}{(\sinh(\beta/2N + \eta))^{2LN}} \times \langle \Psi_0 | (t(-\beta/2N)t(-\eta + \beta/2N))^N | \Psi_0 \rangle,
$$

(3.9)

where

$$
\beta = 2 \sinh(\eta)s.
$$

(3.10)

The expression on the rhs of (3.9) can be interpreted as the partition function of the six-vertex model with inhomogeneities and boundary conditions as given in figure 5. The transfer matrices in (3.9) correspond to adding one more row in the diagram: they generate the imaginary time evolution in the vertical direction.

This specific partition function can be evaluated alternatively by introducing a new transfer matrix which acts in the other direction. This is most easily achieved by performing a reflection along the north-west diagonal (leaving the six vertex weights invariant), leading to the partition function depicted in figure 6. Here the horizontal lines define the action of the so-called quantum transfer matrix (shown in figure 3)

$$
T^{QTM}(u) = L_{2N,0}(u + \beta/2N)L_{2N-1,0}(u - \beta/2N + \eta) \cdots L_{2,0}(u + \beta/2N)
$$

$$
\times L_{1,0}(u - \beta/2N + \eta).
$$

In the standard problem of the thermodynamics of the spin chain a similar partition function is obtained with periodic boundary conditions in both directions. Therefore in that case the trace of $T^{QTM}$ in auxiliary space needs to be taken. However, for the quench problem considered here the boundary conditions on the left and right sides are non-trivial. This leads to

$$
\langle \Psi_0 | \exp(-sH) | \Psi_0 \rangle = \lim_{N \to \infty} \text{Tr} \ T^{L/2}/2,
$$

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\[ |\psi\rangle \otimes |\psi\rangle \otimes \cdots \otimes |\psi\rangle \]

**Figure 5.** The special partition function of the six-vertex model which generates the Trotter decomposition of (2.2). There are \(2N\) horizontal lines with rapidities equal to 0, and \(L\) vertical lines with rapidities \(a_1 = \beta/2N\) and \(a_2 = -\beta/2N + \eta\).

where

\[ \mathcal{T} = \frac{\langle v|T_{QTM}^0(0) \otimes T_{QTM}^0(0)|v\rangle}{(\sinh(-\beta/2N + \eta))^{4N}}. \]  

(3.11)

The scalar product in (3.11) is to be understood as the tensor product of two auxiliary spaces. We call the operator \(\mathcal{T}\) the boundary quantum transfer matrix.

Denoting the eigenvalues of \(\mathcal{T}\) by \(\Lambda_j\),

\[ \langle \Psi_0 | \exp(-sH) | \Psi_0 \rangle = \lim_{N \to \infty} \sum_{j=1}^{2^{2N}} (\Lambda_j)^{L/2}. \]  

(3.12)

In analogy with the periodic case [31] we make the following assumptions.

- There is a leading eigenvalue \(\Lambda\) which remains separated from the others by a finite amount even in the \(N \to \infty\) limit.
- The large \(L\) behaviour of (3.12) can be studied by exchanging the limits \(N \to \infty\) and \(L \to \infty\).

The first assumption is justified by numerical checks (see below), whereas we accept the second one based on experience with the periodic case. Then the large volume behaviour is dominated by the leading eigenvalue

\[ \langle \Psi_0 | \exp(-sH) | \Psi_0 \rangle \approx \left( \lim_{N \to \infty} \Lambda \right)^{L/2}. \]
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Figure 6. The partition function after a reflection along the north-west diagonal. The rapidity associated with the horizontal lines is 0. The rapidities along the vertical lines are $a_1 = -\beta/2N$ and $a_2 = \beta/2N - \eta$. The time evolution in the vertical direction is generated by the boundary quantum transfer matrix (3.11), which adds two horizontal lines together with the boundary conditions specified by $\langle v |$ and $| v \rangle$.

Finally,

$$g(s) = \lim_{L \to \infty} \frac{1}{L} \log \langle \Psi_0 | \exp(-sH) | \Psi_0 \rangle = \frac{1}{2} \lim_{N \to \infty} \log \Lambda.$$

The remaining task is to diagonalize $T$ and find its leading eigenvalue in the Trotter limit. This can be achieved within the framework of the boundary algebraic Bethe Ansatz.

4. The boundary algebraic Bethe Ansatz

The boundary algebraic Bethe Ansatz was developed by Sklyanin in [32] to diagonalize Hamiltonians of open spin chains with possible boundary magnetic fields. Here we use this technology to diagonalize the boundary quantum transfer matrix. For a detailed explanation of the method we refer the reader to [33].

The boundary transfer matrix of a generic inhomogeneous spin chain of length $M$ is defined as

$$R(u) = \text{Tr}_0 \{ K^+(u)T_1(u)K^-(u)T_2(u) \}.$$  \hspace{1cm} (4.1)

Here

$$T_1(u) = \tilde{L}_M(u) \cdots \tilde{L}_1(u),$$
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where \( \tilde{L}_j(u) \) are local Lax-operators given by

\[
\tilde{L}_j(u) = R_{0j}(u - \xi_j)
\]

and

\[
T_2(u) = \gamma(u)\sigma^u_0 T_1^0(-u)\sigma^v_0,
\]

where \( \gamma(u) = (-1)^M \). In the following \( M \) is always even so we are free to set \( \gamma = 1 \). The parameters \( \xi_j \) are the inhomogeneities along the chain. The boundary transfer matrix is depicted in figure 4.

For the \( K \)-matrices entering (4.1) we choose the diagonal solution to the reflection equation \([32, 33]\),

\[
K^\pm(u) = K(u \pm \eta/2, \xi \pm) \quad \text{with} \quad K(u, \xi) = \begin{pmatrix}
\sinh(\xi + u) & 0 \\
0 & \sinh(\xi - u)
\end{pmatrix},
\]

(4.3)

Introducing the components of \( T_1 \) in auxiliary space as usual,

\[
T_1(u) = \begin{pmatrix}
A(u) & B(u) \\
C(u) & D(u)
\end{pmatrix},
\]

(4.4)

the boundary transfer matrix can be written as

\[
\mathcal{R}(u) = k_1^+ k_1^- A(u) D(-u) - k_1^- k_2^+ B(u) C(-u) - k_2^+ k_1^- C(u) B(-u) + k_2^+ k_2^- D(u) A(-u),
\]

(4.5)

where

\[
k_\pm^a \equiv K^\pm_{aa}
\]

are the diagonal elements of the \( K \)-matrices.

The formula (4.5) is equivalent to

\[
\mathcal{R}(u) = \langle v^+(u) | T_1(u) \otimes T_1(-u) | v^-(u) \rangle,
\]

(4.6)

where

\[
|v^-(u)\rangle = k_1^-(u)|+\rangle - k_2^-(u)|-\rangle \quad \langle v^+(u)\rangle = k_1^+(u)\langle + | - k_2^+(u)\langle - |.
\]

(4.7)

Setting \( u = 0 \) gives

\[
\mathcal{R}(0) = \langle v^+ | T_1(0) \otimes T_1(0) | v^- \rangle
\]

(4.8)

with

\[
|v^-\rangle = \sinh(\xi^- - \eta/2)|+\rangle - \sinh(\xi^- + \eta/2)|-\rangle \\
\langle v^+\rangle = \sinh(\xi^+ + \eta/2)\langle + | - \sinh(\xi^+ - \eta/2)\langle - |.
\]

(4.9)

The boundary transfer matrix (4.8) is proportional to the operator \( T \) of (3.11) if the following identifications are made.

- \( M = 2N \).
- The inhomogeneities are \( \xi_{2j+1} = -\beta/2N \), \( \xi_{2j} = \beta/2N - \eta \).
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- The parameters $\xi^\pm$ of the $K$-matrices are determined by

$$
\gamma = \frac{\sinh(\xi^- + \eta/2)}{\sinh(\xi^- - \eta/2)} = \frac{\sinh(\xi^+ - \eta/2)}{\sinh(\xi^+ + \eta/2)}. \tag{4.10}
$$

If the above conditions hold then

$$
\mathcal{T} = \frac{1}{(\sinh(-\beta/2N + \eta))^{4N}} \frac{1}{\langle v^+ | v^- \rangle} \mathcal{R}(0). \tag{4.11}
$$

The common eigenstates of the operators $\mathcal{R}$ can be created from the ferromagnetic reference state $|F\rangle = |++ \cdots\rangle$ as

$$
|\{\lambda\}_n\rangle = \prod_{j=1}^n \mathcal{B}_-(\lambda_j) |F\rangle, \tag{4.12}
$$

where the $\mathcal{B}_-(\lambda)$ operators are defined through

$$
\mathcal{U}_-(\lambda) = T_1(\lambda) K^-(\lambda) T_2(\lambda) = \begin{pmatrix} \mathcal{A}_-(u) & \mathcal{B}_-(u) \\ \mathcal{C}_-(u) & \mathcal{D}_-(u) \end{pmatrix}.
$$

The states in (4.12) are eigenstates if the rapidities satisfy the Bethe equations

$$
\left[ \frac{\sinh(\lambda_j + \beta/2N - \eta)}{\sinh(\lambda_j - \beta/2N + \eta)} \right]^{2N} \prod_{k \neq j} \frac{\sinh(\lambda_j - \lambda_k + \eta)}{\sinh(\lambda_j - \lambda_k - \eta)} \frac{\sinh(\lambda_j + \lambda_k + \eta)}{\sinh(\lambda_j + \lambda_k - \eta)} 
\times \frac{\sinh(\lambda_j - (\xi^- - \eta/2)) \sinh(\lambda_j - (\xi^- - \eta/2))}{\sinh(\lambda_j + (\xi^- - \eta/2)) \sinh(\lambda_j + (\xi^- - \eta/2))} = 1. \tag{4.13}
$$

For every set of Bethe roots $\{\lambda\}_n$ it is useful to introduce the doubled set $\{\tilde{\lambda}\}_{2n} = \{\lambda\}_n \cup \{-\lambda\}_n$. Then the Bethe equations read

$$
\left[ \frac{\sinh(\lambda_j + \beta/2N - \eta)}{\sinh(\lambda_j - \beta/2N + \eta)} \right]^{2N} \prod_{k=1}^{2n} \frac{\sinh(\lambda_j - \tilde{\lambda}_k + \eta)}{\sinh(\lambda_j - \tilde{\lambda}_k - \eta)} 
\times \frac{\sinh(\lambda_j - (\xi^- - \eta/2)) \sinh(\lambda_j - (\xi^- - \eta/2)) \sinh(2\lambda_j - \eta)}{\sinh(\lambda_j + (\xi^- - \eta/2)) \sinh(\lambda_j + (\xi^- - \eta/2)) \sinh(2\lambda_j + \eta)} = -1. \tag{4.14}
$$

The eigenvalues $\Lambda(u, \{\lambda\}_n)$ of the transfer matrix $\mathcal{R}(u)$ are given by

$$
\Lambda(u) = \frac{1}{\sinh(2u)} \left[ \sinh(2u + \eta) \sinh(u + \xi^- - \eta/2) \sinh(u + \xi^- - \eta/2) \right. 
\times \left( \frac{\sinh(u - \beta/2N + \eta)}{\sinh(u + \beta/2N)} \right)^{2N} \prod_{k=1}^{2n} \frac{\sinh(u - \tilde{\lambda}_k - \eta)}{\sinh(u - \tilde{\lambda}_k + \eta)} 
\times \sinh(2u - \eta) \sinh(u + \xi^- + \eta/2) \sinh(u + \xi^- + \eta/2) 
\times \left. \frac{\sinh(u - \beta/2N - \eta)}{\sinh(u - \beta/2N)} \right)^{2N} \prod_{k=1}^{2n} \frac{\sinh(u - \tilde{\lambda}_k + \eta)}{\sinh(u - \tilde{\lambda}_k - \eta)}. \tag{4.15}
$$

These equations are the basis for analysing the leading eigenvalue $\Lambda$ of the operator $\mathcal{T}$. In section 5 we focus on the particular case of the Néel state for generic $\Delta$. In section 6 the case of the dimer state is considered for $\Delta = 1$. 

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5. Boundary QTM: the Néel state

Putting

\[ \xi^- = -\eta/2, \quad \xi^+ = \eta/2 \]

into (4.9) leads to

\[ |v^-\rangle = -\sinh(\eta)|+\rangle \quad \langle v^+| = \sinh(\eta)+| -\rangle. \quad (5.1) \]

These two-site states generate the Néel state with the normalization following from

\[ \langle v^+|v^-\rangle = -\sinh^2(\eta). \quad (5.2) \]

From (4.14) follow the Bethe equations

\[ K(\lambda_j) \left[ \frac{\sinh(\lambda_j + \beta/2N - \eta) \sinh(\lambda_j - \beta/2N)}{\sinh(\lambda_j - \beta/2N + \eta) \sinh(\lambda_j + \beta/2N)} \right]^{2N} \prod_{k=1}^{2n} \frac{\sinh(\lambda_j - \tilde{\lambda}_k + \eta)}{\sinh(\lambda_j - \tilde{\lambda}_k - \eta)} = -1 \quad (5.3) \]

with

\[ K(u) = \frac{\sinh(u + \eta) \sinh(2u - \eta)}{\sinh(u - \eta) \sinh(2u + \eta)}. \]

The eigenvalues of \( \mathcal{R}(u) \) at \( u = 0 \) take the remarkably simple form

\[ \Lambda(0) = -\sinh^2(\eta)(\sinh(\beta/2N + \eta) \sinh(\beta/2N))^{2N} \prod_{k=1}^{2n} \frac{\sinh(\tilde{\lambda}_k + \eta)}{\sinh(\tilde{\lambda}_k)}. \quad (5.4) \]

These equations will be analysed further in the case of \( \Delta > 1 \) corresponding to \( \eta \in \mathbb{R} \). Experience with the periodic case suggests that at any finite \( N \) the leading eigenvalue will be given by a state with \( N \) Bethe roots which are all situated at the imaginary axis. We checked that this is indeed true. We constructed the matrix \( \mathcal{R}(0) \) using the computer program octave and diagonalized it numerically for small systems of \( N = 2, 4, 6, 8 \). We searched for the unique solution of (5.3) with \( N \) roots at the imaginary axis. Computing (5.4) we found exact agreement with the result of exact diagonalization. Moreover, we found that the behaviour of the next to leading eigenvalue is consistent with a non-vanishing gap in the \( N \to \infty \) limit.

Collecting the normalization factors the leading eigenvalue of \( T \) is

\[ \Lambda = \left( \frac{\sinh(\beta/2N)}{\sinh(\eta - \beta/2N)} \right)^{2N} \prod_{k=1}^{2n} \frac{\sinh(\tilde{\lambda}_k + \eta)}{\sinh(\tilde{\lambda}_k)}. \quad (5.5) \]

Solving the Bethe equations showed that the behaviour of the roots as a function of \( N \) is the same as in the periodic case: they cluster around \( u = 0 \) but they do not become dense at any \( u \neq 0 \); all roots have a finite limit as \( N \to \infty \).

5.1. Taking the Trotter limit

We define the auxiliary function

\[ a(u) = K(u) \left[ \frac{\sinh(u + \beta/2N - \eta) \sinh(u - \beta/2N)}{\sinh(u - \beta/2N + \eta) \sinh(u + \beta/2N)} \right]^{2N} \prod_{k=1}^{2n} \frac{\sinh(u - \tilde{\lambda}_k + \eta)}{\sinh(u - \tilde{\lambda}_k - \eta)}. \quad (5.6) \]

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Also, we define
\[ A(u) = \frac{1 + a(u)}{1 + K(u)}. \] (5.7)

Both functions are $i\pi$ periodic.

We define the canonical contour $C$ just as in the periodic case: it has to encircle all Bethe roots but no additional zeros of $1 + a(u)$ [31]. For $\Delta > 1$ the contour can be chosen to consist of two vertical line segments running from $\alpha - i\pi/2$ to $\alpha + i\pi/2$ and from $-\alpha + i\pi/2$ to $-\alpha - i\pi/2$. Here $\alpha \in \mathbb{R}$ is an arbitrary parameter satisfying $\alpha < \eta/2$.

The analytic properties of $A(u)$ inside the contour $C$ are as follows.

- It has an $2N$th order pole at $u = \beta/2$.
- It has $2N$ zeros at the (doubled set of) Bethe roots $\tilde{\lambda}_j$.
- It has no additional zeros or poles; therefore its winding number is zero and its logarithm can be defined to be single valued.

Note that $1 + a(u)$ has an extra zero at $u = i\pi/2$; however, this is cancelled by the denominator of (5.7). We checked with Mathematica that for the solutions of the Bethe equations with $n = N$ there are indeed no other zeros within the canonical contour.

For any function $f(\omega)$ which is analytic within the contour the following holds:
\[ \int_C \frac{d\omega}{2\pi i} f'(\omega) \log(A(\omega)) = 2N f(-\beta/2N) - \sum_{j=1}^{2N} f(\tilde{\lambda}_j). \]

Taking
\[ f(\omega) = \log \frac{\sinh(u - \omega + \eta)}{\sinh(u - \omega - \eta)} \]
leads to the non-linear integral equation (NLIE)
\[ \log a(u) = \log(K(u)) + 2N \log \left( \frac{\sinh(u - \beta/2N) \sinh(u + \beta/2N + \eta)}{\sinh(u + \beta/2N) \sinh(u - \beta/2N + \eta)} \right) \]
\[ - \int_C \frac{d\omega}{2\pi i} \sinh(2\eta) \frac{\sinh(u - \omega + \eta) \sinh(u - \omega - \eta)}{\sinh(2\eta) \sinh(\omega) \sinh(\omega + \eta)} \log(A(\omega)). \]

Similarly,
\[ \log \Lambda = \int_C \frac{d\omega}{2\pi i} \frac{\sinh \eta}{\sinh(\omega) \sinh(\omega + \eta)} \log(A(\omega)). \]

Here we also used the fact that $\log(A(0)) = 0$.

The above equations are valid at any $N$ and they have a well-behaving Trotter limit. For the auxiliary function we obtain
\[ \log a(u) = \log(K(u)) - 4s \frac{\sinh^2 \eta}{\sinh(u) \sinh(u + \eta)} \]
\[ - \int_C \frac{d\omega}{2\pi i} \frac{\sinh(2\eta)}{\sinh(u - \omega + \eta) \sinh(u - \omega - \eta)} \log(A(\omega)), \quad (5.8) \]
where we used the relation (3.10).
Finally, for the dynamical free energy density we obtain
\[
g(s) = \frac{1}{2} \log \Lambda = \frac{1}{2} \int \frac{d\omega}{2\pi i} \frac{\sinh \eta}{\sinh(\omega + \eta)} \log(A(\omega)). \tag{5.9}
\]
Equations (5.8) and (5.9) constitute the main result of this section. They are valid for any \(s \in \mathbb{R}^+\) and they can be used as a basis for the analytic continuation \(s = it\) which is investigated in section 5.4.

5.2. The small \(s\) limit

It is useful to check the \(s \to 0\) limit of the NLIE analytically, as this provides a non-trivial check of the calculations. The solution of the NLIE at \(s = 0\) is
\[
a(u) = K(u) \quad A(u) = 1,
\]
which gives \(g(0) = 0\) as it should by its definition.

The first order term in \(g(s)\) is expected to be the Hamiltonian density
\[
g(s) = -\frac{\langle N|H|N \rangle}{L} = 2 \cosh \eta. \tag{5.10}
\]
In the following we derive this result from the NLIE. We define
\[
a'(u) = \frac{1}{a(u)} \frac{\partial a(u)}{\partial s}.
\]
This function satisfies the linear integral equation
\[
a'(u) = -4 \frac{\sinh^2 \eta}{\sinh(u) \sinh(u + \eta)} - \int \frac{d\omega}{2\pi i} \frac{\sinh(2\eta)}{\sinh(u - \omega + \eta) \sinh(u - \omega - \eta)} \frac{a'(u)a(u)}{1 + a(u)}.
\]
The solution at \(s = 0\) can be obtained by simple contour integrals, leading to
\[
a'(\lambda) = 4 \frac{\sinh^2(\eta) \cosh(\lambda)}{\sinh(\lambda) \sinh(\lambda - \eta) \sinh(\lambda + \eta)}.
\]
Finally, we obtain
\[
\frac{\partial g}{\partial s} \bigg|_{s=0} = \int_C \frac{d\omega}{2\pi i} \frac{\sinh^2 \eta}{\sinh(\omega + \eta) \sinh(\omega + \eta)} \frac{a'(\omega)}{1 + K(-u)}
\]
\[
= \int_C \frac{d\omega}{2\pi i} \frac{2\sinh^4 \eta \cosh(\omega)}{\sinh^2(\omega + \eta) \sinh(\omega + \eta) \sinh(\omega - \eta)}
\]
\[
\times \frac{\sinh(2u - \eta)}{\sinh(u + \eta) \sinh(2u - \eta) + \sinh(u - \eta) \sinh(2u + \eta)} = 2 \cosh \eta.
\]
It is also possible to derive the higher order terms from the NLIE by taking further derivatives and solving linear equations. However, this becomes very cumbersome already for the second cumulant, so in practice it is more convenient to determine them from explicit real-space calculations. For the sake of completeness we give here the second cumulant,
\[
\kappa_2 = \frac{\langle N|H^2|N \rangle - \langle N|H|N \rangle^2}{L} = 4. \tag{5.11}
\]
5.3. The large $s$ limit

At large positive $s$ the behaviour of $g(s)$ will be determined by the low lying states of the antiferromagnetic Hamiltonian. In the $\Delta > 1$ regime considered here the two lowest lying states of the Hamiltonian $|\text{GS}_1\rangle$ and $|\text{GS}_2\rangle$ are such that they become degenerate in the thermodynamic limit with an energy density $e_0$, but a finite gap remains between them and the next state. Therefore in the large $s$ limit we have

$$e^{g(s)L} \approx \left(|\langle N|\text{GS}_1\rangle|^2 + |\langle N|\text{GS}_2\rangle|^2\right) e^{-se_0L}. \quad (5.12)$$

The overlap of the ground states with the Néel state scales as

$$|\langle N|\text{GS}_{1,2}\rangle|^2 = \alpha_{1,2} \exp(\beta_{1,2}L). \quad (5.13)$$

Although the pre-factors $\alpha_1$ and $\alpha_2$ can be different, we expect that the exponent will be the same, $\beta_1 = \beta_2 = \beta$. We checked this by a finite volume numerical investigation, which will be published elsewhere. We call the quantity $e^\beta$ the ‘overlap per site’.

Putting everything together, the large $s$ behaviour of $g(s)$ is

$$g(s) = -e_0s + \beta + \cdots. \quad (5.14)$$

In the following we extract $e_0$ and $\beta$ from the NLIE. First we perform a rotation of $\pi/2$ in the complex plane and introduce

$$\tilde{a}(u) = \frac{a(u)}{K(u)}. \quad (5.15)$$

In this way the NLIE takes the form

$$\log \tilde{a}(\lambda) = s\frac{4 \sinh^2 \eta}{\sin(\lambda) \sin(\lambda - i\eta)} + \int_C \frac{d\omega}{2\pi} \frac{2 \sinh 2\eta}{\sin(\lambda - \omega + i\eta) \sin(\lambda - \omega - i\eta)} \log(A(\omega)) \quad (5.16)$$

with

$$A(u) = \frac{1 + K(u)\tilde{a}(u)}{1 + K(u)}. \quad (5.17)$$

The integration contour consists of two horizontal line segments

$$C^+ = [-\pi/2 + i\alpha \cdots \pi/2 + i\alpha] \quad \text{and} \quad C^- = [-\pi/2 - i\alpha \cdots \pi/2 - i\alpha]. \quad (5.18)$$

For the dynamical free energy we obtain

$$g(s) = -\frac{1}{2} \int_C \frac{d\omega}{2\pi} \frac{\sinh \eta \log(A(\omega))}{\sin(\lambda) \sin(\lambda - i\eta)}. \quad (5.19)$$

Note that as a complex integral $d\omega$ is negative on the upper and positive on the lower contour, i.e. formally we have

$$\int_C \frac{d\omega}{2\pi} = -\int_{C^+} \frac{d\omega}{2\pi} + \int_{C^-} \frac{d\omega}{2\pi},$$

where the integrals on the rhs are to be understood as purely real integrals.

The auxiliary function can be expanded as

$$\log \tilde{a}(\lambda) = s\rho(\lambda) + \kappa(\lambda) + \cdots.$$
Investigating the numerical solutions of the NLIE, we find that the real part of \( \rho \) is positive on the upper contour and negative on the lower contour. Therefore, on the upper contour

\[
\log A(u) \to s\rho(\lambda) + \kappa(\lambda) + \log \frac{K(u)}{1 + K(u)},
\]

whereas on the lower contour

\[
\log A(u) \to \log \frac{1}{1 + K(u)}.
\]

First we compute the linear terms in \( s \) for which only the upper contour contributes. For \( \rho(u) \) we obtain the integral equation

\[
\rho(\lambda) = \frac{4 \sinh^2 \eta}{\sin(\lambda) \sin(\lambda - i\eta)} - \int_{C^+} \frac{d\omega}{2\pi \sin(\lambda - \omega + i\eta) \sin(\lambda - \omega - i\eta)} \rho(\omega).
\]

This integral can be solved in Fourier space and leads to

\[
e_0 = \frac{1}{2} \int_{C^+} \frac{d\omega}{2\pi \sin(\lambda) \sin(\lambda - i\eta)} \rho(\lambda) = 2 \sinh \eta \sum_{n=-\infty}^{\infty} e^{-|n| \cosh(\eta)}.
\]

This is the known formula for the ground state energy of the XXZ chain in the massive regime.

For the sub-leading contributions we need to keep the \( O(1) \) terms from the lower contour too. For \( \kappa(u) \) we obtain the linear equation

\[
\kappa(\lambda) = -\int_{C^+} \frac{d\omega}{2\pi \sin(\lambda - \omega + i\eta) \sin(\lambda - \omega - i\eta)} \kappa(\omega)
- \int_{C^+} \frac{d\omega}{2\pi \sin(\lambda - \omega + i\eta) \sin(\lambda - \omega - i\eta)} \log \frac{K(i\omega)}{1 + K(i\omega)}
- \int_{C^-} \frac{d\omega}{2\pi \sin(\lambda - \omega + i\eta) \sin(\lambda - \omega - i\eta)} \log(1 + K(i\omega)).
\]

Finally, for the exponent \( \beta \) we get

\[
\beta = \frac{1}{2} \int_{C^+} \frac{d\omega}{2\pi \sin(\lambda) \sin(\lambda - i\eta)} \kappa(\omega)
+ \frac{1}{2} \int_{C^+} \frac{d\omega}{2\pi \sin(\lambda) \sin(\lambda - i\eta)} \log \frac{K(i\omega)}{1 + K(i\omega)}
- \frac{1}{2} \int_{C^-} \frac{d\omega}{2\pi \sin(\lambda) \sin(\lambda - i\eta)} \log \frac{1}{1 + K(i\omega)}.
\]

Equations (5.23) and (5.24) can be solved easily in Fourier space; numerical results are shown in table 1. Generally we observe that the overlap per site is a monotonically growing

| \( \Delta \) | 1.01 | 1.1 | 1.5 | 2 | 4 |
|---|---|---|---|---|---|
| \( \exp(\beta) \) | 0.836 021 43 | 0.848 963 60 | 0.902 961 03 | 0.941 683 83 | 0.984 623 08 |

Table 1. The overlap per site between the Néel state and the ground state of the XXZ Hamiltonian for different \( \Delta > 1 \).
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Figure 7. Numerical results for the dynamical free energy density and the Loschmidt echo for $\eta = 0.5$ ($\Delta = 1.1276$). (a) The dynamical free energy density for real $s$. The solid line shows the results of the NLIE, whereas the straight line is the large $s$ asymptotic (5.14). (b) The Loschmidt echo per site for small real times. The squares represent the results of the NLIE, whereas the dashed line shows the quadratic approximation.

function of $\Delta$; in the $\Delta = \infty$ limit it approaches 1 as expected, and it has a finite limit at $\Delta = 1$.

5.4. Numerical results for $g(s)$ and the Loschmidt echo

We numerically implemented the NLIEs (5.8) and (5.9) for $\Delta > 1$ using the computer program octave. As a first step we investigated the behaviour of $g(s)$ for real positive $s$. It was found that the simple iteration technique converges and the results do not depend on the parameter $\alpha$ determining the position of the integration contour. Numerical results (together with the predicted large $s$ asymptotic) are shown in figure 7(a). We also investigated the positions of the zeros of the function $A(u)$ defined by (5.7). It was found that for purely real values of $s$ all zeros lie symmetrically on the imaginary axis, as expected.

As a second step we turned to the problem of analytic continuation. It was found that the NLIE remains stable in a finite neighbourhood of the positive real axis. Giving small imaginary parts to $s$ we observed that the zeros of $A(u)$ move away from the imaginary axis, but they still cluster at $u = 0$. The NLIE remains stable even for $s = it, t \in \mathbb{R}$ up to a certain critical value $t = t^*$. In this case all zeros of $A(u)$ are positioned on the real axis. We observed that the zeros move outwards as $t$ is increased and they approach the contour $C$. The NLIE is valid until all zeros lie within the contour\(^1\), therefore it is useful to choose the maximal value $\alpha = \eta/2 - \epsilon$. However, at the threshold $t = t^*$ the NLIE becomes numerically unstable even before the outermost zero crosses the contour. We found that the critical value is approximately $t^* \approx \eta/(2 \sinh \eta)$. In figure 7(b) we plot

\(^1\) This statement can be proven by the following argument. The zeros of $A(u)$ cluster around $u = 0$, but by fixing a specific zero it can be shown that its position depends continuously on the Trotter number $N$. Therefore, if a zero is outside the canonical contour in the Trotter limit, then this means that there is an $N_c$ such that for all $N > N_c$ it is outside the contour and then the NLIE is not valid anymore.

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the numerical results for the Loschmidt echo per site for \( \eta = 0.5 \) and \( 0 < t < t^\ast \). In this regime the quadratic approximation using the second cumulant (5.11) works very well and it deviates only slightly from the exact result of the NLIE.

Based on the behaviour of the zeros in the regime \( 0 < t < t^\ast \) we expect that for all \( s = it \) they move outwards as \( t \) is increased, and they leave the canonical contour one by one at certain threshold values \( t^\ast_j, j = 1 \cdots \infty \). The structure of the NLIE has to be changed at each of these points to account for the missing zeros.

In the numerical investigations above we assumed that the gap in the BQTM does not vanish and that the leading eigenvalue is always given by the analytic continuation of the same state. This certainly holds if \( s \) is close enough to the real positive axis. However, for general complex \( s \) level crossings can appear which lead to non-analytic behaviour in the dynamical free energy. We plan to address these questions in a future work.

6. Boundary QTM: the XXX limit and the dimer state

In this section we consider the XXX chain where \( \Delta = 1 \). Typically all formulae relevant for the Bethe Ansatz solution of the XXX chain are easily obtained from their XXZ counterparts by a simple \( \eta \rightarrow 0 \) limit and a rescaling of the rapidities by \( \eta^2 \). This is also true for the quantities considered in this work. Here we only give the main equations and do not repeat the whole derivation presented in the previous two sections. We will be mainly concerned with the dimer state, i.e. we calculate \( g(s) \) defined as

\[ e^{g(s) L} = \langle D | e^{-sH} | D \rangle, \]

where

\[ D = \otimes_{j=1}^{L/2} \left( \frac{|+\rangle - |\rangle_\pm}{} \right). \]

The algebraic Bethe Ansatz construction uses the rational \( R \)-matrix

\[ R(u) = \begin{pmatrix} u + i & i \\ u & i \\ i & u \end{pmatrix}. \tag{6.1} \]

The boundary \( K \)-matrices with generic parameters \( \xi \pm \) are

\[ K_\pm = K(\pm \frac{i}{2}, \xi \pm) \quad \text{with} \quad K(u, \xi) = \begin{pmatrix} \xi + u & 0 \\ 0 & \xi - u \end{pmatrix}. \tag{6.2} \]

The main objective is to diagonalize the matrix

\[ \mathcal{T} = \frac{1}{(-i\beta/2N + i)^{2N}} \frac{1}{\langle v^+ | v^- \rangle} R(0), \tag{6.3} \]

2 This is true for formal expressions about individual states or the thermodynamic quantities. The behaviour of correlation functions is of course different, because the XXX chain is critical, whereas the XXZ chain with \( \Delta > 1 \) is massive.
where $R(u)$ is the boundary transfer matrix

$$R(u) = \langle v^+(u) | T_1(u) \otimes T_1(-u) | v^-(u) \rangle. \quad (6.4)$$

The $K$-matrices (6.2) lead to the following two-site boundary states:

$$|v^-\rangle \equiv |v^-(0)\rangle = (\xi^- - i/2) + - \rangle - (\xi^- + i/2) | - \rangle$$

$$\langle v^+| \equiv \langle v^+(0)| = (\xi^+ + i/2) (+ - | - (\xi^+ - i/2) \langle - + |. \quad (6.5)$$

The Bethe Ansatz equations for a set of roots $\{\lambda\}_n$ are

$$\left[ \left( \lambda_j + i\beta/2N - i \right) \left( \lambda_j - i\beta/2N + i \right) \right]^{2N} \prod_{k=1}^{2n} \frac{\lambda_j - \bar{\lambda}_k + i}{\lambda_j - \lambda_k - i}$$

$$\times \frac{\left( \lambda_j - (\xi_+ - i/2) \right) \left( \lambda_j - (\xi_- - i/2) \right) (2\lambda_j - i)}{\left( \lambda_j + (\xi_+ - i/2) \right) \left( \lambda_j + (\xi_- - i/2) \right) (2\lambda_j + i)} = -1 \quad (6.6)$$

and the eigenvalue of $R(u)$ on the given state is

$$\Lambda(u) = \frac{1}{2u} \left[ (2u+i)(u+\xi_+ - i/2)(u+\xi_- - i/2)((u-i\beta/2N+i)(u+i\beta/2N))^{2N} \right.$$

$$\times \prod_{k=1}^{2n} \frac{u - \bar{\lambda}_k - i}{u - \lambda_k}$$

$$\left. + (2u-i)(u-\xi_+ + i/2)(u-\xi_- + i/2)((u+i\beta/2N-i)(u-i\beta/2N))^{2N} \times \prod_{k=1}^{2n} \frac{u - \bar{\lambda}_k + i}{u - \lambda_k} \right]. \quad (6.7)$$

The case of the Néel state is obtained by setting $\xi_- = -i/2$ and $\xi^+ = i/2$. The resulting equations follow from a straightforward limit of the XXZ formulae; therefore we do not consider this case in detail. Instead we focus on the limit

$$\xi_+ \to \infty$$

which produces the dimer states as

$$\lim_{\xi^- \to -\infty} \frac{|v^-\rangle}{\sqrt{2\xi^-}} = \lim_{\xi^+ \to \infty} \frac{|v^+\rangle}{\sqrt{2\xi^+}} = \frac{1}{\sqrt{2}} (|+ - \rangle - |- + \rangle). \quad (6.8)$$

In this limit the Bethe equations become

$$K_D(\lambda_j) \left[ \left( \lambda_j + i\beta/2N - i \right) \left( \lambda_j - i\beta/2N + i \right) \right]^{2N} \prod_{k=1}^{2n} \frac{\lambda_j - \bar{\lambda}_k + i}{\lambda_j - \lambda_k - i} = -1 \quad (6.9)$$

with

$$K_D(u) = \frac{(2u-i)}{(2u+i)}.$$
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The eigenvalues of $T$ are

$$\Lambda = \frac{1}{(-i\beta/2N + i)^{4N}} \lim_{u \to 0} \frac{1}{4u} \left[ (2u + i)((u - i\beta/2N + i)(u + i\beta/2N))^2N \times \prod_{k=1}^{2n} \frac{(u - \tilde{\lambda}_k - i)}{(u - \lambda_k)} + (2u - i)((u + i\beta/2N - i)(u - i\beta/2N))^2N \times \prod_{k=1}^{2n} \frac{(u - \tilde{\lambda}_k + i)}{(u - \lambda_k)} \right].$$

(6.10)

We performed exact diagonalization of $T$ for small values of $N$ and found that the largest eigenvalue is given by the unique state with $N$ purely real roots. Similarly to the XXZ case we define the auxiliary function

$$a(u) = K_D(u) \left[ \frac{(u + i\beta/2N - i)(u - i\beta/2N)}{(u - i\beta/2N + i)(u + i\beta/2N)} \right]^{2N} \prod_{k=1}^{2n} \frac{(u - \tilde{\lambda}_k + i)}{(u - \lambda_k - i)}$$

and

$$A(u) = \frac{1 + a(u)}{1 + K_D(u)}.$$

Also, we define the canonical contour $C$ which now consists of two infinite horizontal lines with imaginary parts $\pm \alpha$ such that $\alpha < 1/2$. The function $A(u)$ has zeros inside the contour given by the (doubled set of) Bethe roots. The trivial zero of $1 + a(u)$ at $u = 0$ is cancelled by the denominator, and further numerical checks showed that for the leading state there are indeed no other zeros inside $C$.

It is now a straightforward exercise to derive an NLIE for the auxiliary function. Here we just give the result valid in the Trotter limit,

$$\log a(\lambda) = \log(K_D(u)) + s \frac{4}{\lambda(\lambda + i)} - \int_C \frac{d\omega}{2\pi} \frac{2}{(\lambda - \omega)^2 + 1} \log(A(\omega)).$$

(6.11)

Expressing the eigenvalue as an integral is more involved because (6.10) is not of a product form. However, the same manipulations which are used in the periodic case [31] can be performed here as well and in the Trotter limit we find

$$g(s) = \lim_{N \to \infty} \log \Lambda \frac{2}{2} = -\frac{1}{2} \int_C \frac{d\omega}{2\pi} \omega \log(A(\omega)).$$

(6.12)

Equations (6.11) and (6.12) are the main results of this section.

For the sake of completeness we note that in the case of the Néel state the same equations apply with the only difference being that the reflection factor $K_D(u)$ has to be replaced by

$$K_N(u) = \frac{(u + i)(2u - i)}{(u - i)(2u + i)}.$$
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6.1. The $s = 0$ limit

At $s = 0$ the solution of the NLIE (6.11) is simply $a(u) = K_D(u)$, and this yields $g(0) = 0$ as expected. As a non-trivial check we compute the expectation value of the Hamiltonian from the NLIE,

$$\langle D|H|D\rangle = -\frac{\partial g}{\partial s} = -\int C \frac{1}{2\pi \omega(\omega + i)} \frac{a'(\omega)}{1 + K_D(-\omega)}.$$

Here $a'(u)$ is the solution of the linear integral equation

$$a'(u) = 4 \frac{u^2 - 1}{u(u^2 + 1)} - \int C \frac{2}{2\pi (u - \omega)^2 + 1} \frac{a'(\omega)}{1 + K_D(-\omega)}.$$

The solution is

$$a'(u) = 4i \frac{u^2 - 1}{u(u^2 + 1)}.$$

This leads to

$$\langle D|H|D\rangle = -\int C \frac{1}{2\pi u(u + i)} \frac{u^2 - 1}{u(u^2 + 1)} \frac{2u - i}{u} = -\frac{5}{2}.$$

It can be checked by a straightforward real-space calculation that this is indeed the correct expectation value.

6.2. The $q$-deformed dimer state

The natural generalization of the dimer state to $\Delta \neq 1$ is the so-called $q$-deformed dimer state

$$|qD\rangle = \bigotimes_{j=1}^{L/2} \left( \frac{|+\rangle - q|\rangle}{\sqrt{1 + q^2}} \right),$$

where $\Delta = (q + 1/q)/2$. This state (together with its translation by a site one) is the ground state of the $q$-deformed Majumdar–Ghosh Hamiltonian derived in [34].

Consider the function $g(s)$ defined as

$$e^{g(s)L} = \langle qD|e^{-sH}|qD\rangle,$$

where the anisotropy $\Delta$ of the Hamiltonian is the same as that of the initial state. Based on the previous calculations it is easy to see that equations (5.8) and (5.9) hold also in this case with

$$K(u) = \frac{\sinh(2u - \eta)}{\sinh(2u + \eta)}.$$

7. Conclusions

In this work we derived exact analytical results for the dynamical free energy density (the Loschmidt echo for imaginary times) for certain quantum quenches in the XXZ spin chain. As initial states we considered the Néel state and the $q$-deformed dimer state, which are both products of local two-site states. In all cases considered the resulting equation for
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The dynamical free energy takes the form

\[ g(s) = \frac{1}{2} \int_C \frac{d\omega}{2\pi i} \tilde{e}(u) \log \left( \frac{1 + a(u)}{1 + K(u)} \right), \]  

where \( a(u) \) is the solution of the NLIE

\[ \log a(u) = \log(K(u)) - 2se(u) - \int_C \frac{d\omega}{2\pi i} \varphi(u - \omega) \log \left( \frac{1 + a(u)}{1 + K(u)} \right). \]

The function \( e(u) \) is a function related to the one-particle energy (differing from \( \tilde{e}(u) \) by a simple proportionality factor), \( \varphi(u) \) is the one-particle scattering kernel, and the complex contour \( C \) depends on the anisotropy \( \Delta \). The difference between these equations and those describing the thermodynamic free energy density [31] is the appearance of the extra source term \( \log(K(u)) \) (which carries the information about the initial state) and the regulator \( 1/(1 + K(u)) \) for the integrals which was introduced to correctly handle the zeros of the function \( 1 + a(u) \).

We observed that the NLIE is numerically stable in a finite neighbourhood of the real positive axis including the purely imaginary values \( s = it \) with small \( t \in \mathbb{R} \); therefore it is capable of providing exact results for the Loschmidt echo per site. We found that as \( t \) is increased the zeros of the function \( 1 + a(u) \) move outwards from the origin, and increasing \( t \) further they would eventually cross the canonical contour. In this case the equations have to be modified accordingly. However, the NLIE becomes numerically unstable even before the first crossing appears, and further work is needed to obtain numerical data for larger real times. Also, it needs to be checked whether and in what cases level crossings of the boundary quantum transfer matrix occur at real times, which could lead to non-analyticity of the Loschmidt echo. We plan to return to these questions in a future work.

The reason for choosing the Néel state and the \((q\text{-deformed})\) dimer state was that in these cases the additional zero of the function \( 1 + a(u) \) within the canonical contour which does not correspond to a Bethe root is fixed to \( u = i\pi/2 \) or \( 0 \). In the case of

\[ |\Psi_0\rangle = \otimes_{j=1}^{L/2} \left| + + \right> + \gamma \left| - - \right> \]

with arbitrary \( \gamma \) the position of the additional zero depends on both \( s \) and \( \gamma \). In this case a different NLIE can be written down which accounts for the movement of the additional zero.

More general two-site states could be considered by taking off-diagonal \( K \)-matrices for the construction of the boundary transfer matrix (4.1). The diagonalization of these transfer matrices could be achieved using the recent results of [35, 36].

It is an intriguing question whether generalizations of the present methods could lead to analytic expressions for the time-dependent local correlation functions, possibly through a limit

\[ O(t) = \lim_{\beta \to 0} \langle \Psi_0 | e^{(i\beta - i\beta)H} O e^{(-i\beta - i\beta)H} | \Psi_0 \rangle. \]

Results for dynamical correlation functions at equilibrium are already available with the QTM method [37], but it is not evident whether such methods could work for the boundary QTM relevant to the quench problem. While it is straightforward to translate the rhs of (7.4) to a six-vertex model partition function and the leading state of the relevant
The dynamical free energy and the Loschmidt echo for a class of quantum quenches in the Heisenberg spin chain boundary quantum transfer matrix could be constructed using the methods of the present work, the insertion of the local operators leads to scalar products whose evaluation is very challenging even at finite Trotter number.

While this work was being finished, the paper [25] appeared where Fagotti derived a different NLIE for \( g(s) \) using the GGE hypothesis for the exponential of the Hamiltonian. While the source term of the NLIE of [25] is not explicit (the Lagrange-multipliers are not specified), analytical or numerical results could still be obtained for small quenches, for example using a \( 1/\Delta \) expansion for the quench starting from the Néel state. Also, it was observed in [25] that the winding number of the auxiliary function changes as the time \( t \) is increased. This is in complete accordance with the movement of the zeros of \( A(u) \) observed in the present work.

We believe that it is worthwhile to stress the differences between our results and those of [25]. Our lattice path integral derivation of \( g(s) \) is based on first principles, the assumptions about the analyticity of the auxiliary functions were checked numerically at finite and infinite Trotter number, and we did not make use of the GGE hypothesis. Therefore our NLIE gives an exact result for \( g(s) \) for any \( s \in \mathbb{R}^+ \) and both the source term \( \log(K(u)) \) and the regulator \( 1/(1 + K(u)) \) are explicit. On the other hand, the analytic continuation to real times \( (s = it) \) and in general the behaviour of \( g(s) \) for complex \( s \) deserves further study. Also, it is an interesting question whether there is a direct relation between our NLIE and that of [25]. Comparison of our numerical results with those of [25] could lead to a first check of the GGE hypothesis for the XXZ spin chain. These questions are left for future research.

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