Exact boundary free energy of the open XXZ chain with arbitrary boundary conditions

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Abstract. We derive an exact formula for the boundary free energy of the open Heisenberg XXZ spin chain. We allow for arbitrary boundary magnetic fields, but assume zero bulk magnetization. The result is completely analogous to earlier formulas for the so-called γ-function: it is expressed as a combination of single integrals and two simple Fredholm determinants. Our expressions can be evaluated easily using numerical algorithms with arbitrary precision. We demonstrate that the boundary free energy can show a wide variety of behaviour as a function of the temperature, depending on the anisotropy and the boundary fields. We also compute the low temperature limit of the boundary free energy, and reproduce the known results for the ground state boundary energy, including the case of non-diagonal fields.

Keywords: integrable spin chains and vertex models, quantum integrability (Bethe ansatz), thermodynamic Bethe ansatz
1. Introduction

One dimensional integrable quantum models are a special class of many-body systems, that can be solved exactly [1]. The expression ‘exact solution’ usually means that the eigenvalues of the Hamiltonian can be found without approximation, and this is typically performed by one of the forms of the Bethe ansatz. However, integrability also offers powerful tools to investigate physical quantities beyond the spectrum, such as thermodynamical state functions or physical correlation functions, in or out of equilibrium. The calculation of such composite quantities is considerably more involved than simply finding the spectrum.

An area that has attracted continued interest is the integrability of open systems, and the calculation of boundary effects on the physical quantities. The seminal work
of Gaudin on the 1D Bose gas with open boundaries [2] showed that open systems can also be treated with the Bethe ansatz method, and the algebraic foundation for boundary integrability was later given in the classic papers of Cherednik and Sklyanin [3, 4]. The key algebraic component is the so-called boundary Yang–Baxter (BYB) relation or ‘reflection equation’, which guarantees the commutativity of boundary transfer matrices. This relation plays the same role as the reflection relations in factorized scattering theory [3, 5], and each solution to the BYB equations corresponds to a specific integrable boundary condition. In the lattice models the physically relevant solutions (those that act as scalars on the physical Hilbert-space) are called $K$-matrices, and they describe boundary magnetic fields. The eigenstates of such integrable Hamiltonians are then found either by the boundary algebraic Bethe ansatz [4], or by alternative methods such as the separation of variables method [6, 7] (see also [8] and references therein) or closely related analytical approaches [9].

A paradigmatic model of one dimensional magnetism is the $SU(2)$-symmetric Heisenberg spin chain and its anisotropic variants. Whereas the periodic system is solved by the original Bethe ansatz [10], the treatment of the open chain is more involved. In the case of longitudinal boundary magnetic fields (including free boundary conditions) the coordinate Bethe ansatz solution was already given in [11], with the algebraic formulation later supplied in [4]. The relatively simple solution in this case made it possible to derive the boundary contributions to the ground state energy [12, 13].

The longitudinal fields conserve the $U(1)$-symmetry of the model, which is reflected by the existence of a proper reference state; the corresponding solution of the BYB equation is given by the diagonal $K$-matrices. It was later found in [14] that there is a 3-parameter family of $K$-matrices that solve the BYB equations, and the open XXZ spin chain is integrable with arbitrary boundary magnetic fields. The solution of the general non-diagonal case was later given by different groups in a series of works [8, 15–22]. It is now known that the characterization of the transfer matrix spectrum strongly depends on the boundary condition: the so-called T-Q equations include an inhomogeneous term, which is zero only if the two sets of boundary parameters satisfy a special constraint [15, 16]. The inhomogeneous T-Q equations pose considerable challenges in the thermodynamic limit [23], yet it was possible to derive the boundary energy to the ground state using various tricks in a series of works [9, 24, 25], both for the massive and massless regimes of the spin chain.

Having found the characterization of the spectrum, a second step in solving a model can be the computation of its thermodynamic properties. In integrable models the free energy density in the infinite volume limit can be calculated by the so-called Thermodynamic Bethe ansatz (TBA) method [26, 27]. In the XXZ spin chain this leads to a coupled set of non-linear integral equations (NLIE’s), where the number of the nodes depends on the anisotropy parameter [28–30]. In the generic case (including the isotropic point) one gets an infinite set of TBA equations. An alternative way to describe the thermodynamics is the so-called quantum transfer matrix (QTM) method [31, 32], which (for the XXZ chain) leads to a single NLIE over a certain contour in the complex plain. The QTM method is thus preferable for most problems; its equivalence to the TBA was shown in [33].
It is a very natural idea to compute also the boundary free energy (the $O(L^0)$ contribution of a single boundary to the free energy) using the exact methods of integrability. The study of this quantity was initiated in the classic paper of Affleck and Ludwig [34], where it was called the $g$-value (or $g$-function) or ‘non-integer ground state degeneracy’. It was conjectured in [34] and later proven in [35] that the $g$-function always decreases under renormalization group flow and its fixed points coincide with the $g$-values in the corresponding boundary conformal field theories (CFT’s).

Early attempts to derive the $g$-function in the TBA framework led to partial results [36–38], whereas an exact formula was conjectured in [39] based on a low-temperature expansion in massive QFT. It was later shown in [40, 41] that this exact $g$-function can be derived by taking into account both the density of states in rapidity space and the fluctuations around the saddle point solution of the TBA. The general principles behind the $g$-function were thus settled, nevertheless the result has not been applied to the XXZ spin chains. The formalism of [40, 41] would lead to Fredholm determinants that act in rapidity space and also in the infinite dimensional string space, and their numerical or analytical evaluation are expected to be cumbersome. We should note that there had been papers dealing with the boundary free energy of the XXZ chain within the TBA approach [42–44], but they did not include the boundary independent Fredholm determinants that were derived only in [40, 41], and thus they lead to disagreement with field theory calculations [45–47].

The computation of the boundary free energy within the QTM formalism was initiated in [48], and continued in [49], where the $O(1)$ term was expressed as overlaps of the dominant state of the QTM with the boundary states corresponding to the given integrable boundary condition, in complete analogy with the picture in CFT and massive QFT [34, 39]. However, the final exact result of [49] only applied to diagonal boundary conditions, and it was not convenient for further analytical or numerical investigation, as it involved a complicated integral series. The TBA results [40, 41] together with the known parallel between the TBA and QTM suggest that the boundary free energy should be expressed as a combination of single integrals and simple Fredholm determinants, which in the QTM would always be one dimensional (without string indices).

This is the goal that we set in the present paper, and we derive the result for generic boundary magnetic fields. Our starting point is the formulation of the problem laid out in [48, 49], which we here supplement with more recent developments about the relevant scalar products [50–52].

The structure of the paper is as follows. In section 2 we introduce the model and our basic tools. The scalar products central to the work are investigated in section 3. In section 4 we derive the main results for the boundary free energy and the boundary magnetization, and we also treat a number of specific cases. In sections 5 and 6 we investigate the high and low temperature limits. Section 7 includes the formulas specific to the XXX model, whereas in section 8 we treat the ferromagnetic XXZ spin chain. Examples for the numerical data is presented in section 9, together with a comparison to exact diagonalization. Finally, section 10 includes our concluding remarks and the discussion of the open problems.
2. The boundary free energy in the quantum transfer matrix method

2.1. Defining the model and the problem

We define the Hamiltonian of the open anti-ferromagnetic XXZ spin chain as

\[ H = \sum_{j=1}^{L-1} \{ \sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta (\sigma_j^z \sigma_{j+1}^z - 1) \} + \sum_{a=x,y,z} h_a (\sigma_1^a + \sigma_L^a), \]  
(2.1)

where \( \sigma^a \) are the Pauli matrices, and \( h^a \) are the boundary magnetic fields. For simplicity we chose to have the same magnetic fields at the two ends. This is convenient because the contribution of a single boundary will be given by half of the total boundary free energy. Having two different fields would not give a different physical behaviour, because we are taking the infinite length limit when the two ends of the chain completely decouple.

In most of this work we restrict ourselves to \( \Delta > 0 \), but in section 8 we also treat the \( \Delta < 0 \) regime, which (for \( \Delta \leq -1 \)) describes the ferromagnetic chain.

In order to obtain the boundary free energy and to compare it with previous results it is important to fix all additive constants in the Hamiltonian. Therefore we stress that (2.1) is defined such that in the absence of the boundary fields the ferromagnetic states with all spins up (or down) are eigenstates with zero energy.

It is important that we did not include a bulk magnetic field in the Hamiltonian. The addition of a term \( H' = h \sum_{j=1}^{L} \sigma_j^z \) is compatible with integrability if the boundary fields are also longitudinal \( (h_x = h_y = 0) \). However, our current mathematical tools can only be applied to the case of \( h = 0 \); the reasons for this will be explained in the Conclusions. On the other hand, we are able to treat the case of general boundary fields, which is an advantage of our methods. In these cases \( H' \) does not commute with the Hamiltonian, therefore the bulk magnetic field would spoil integrability. In conclusions we give further comments about this issue.

We note that the case of free boundary conditions is the most relevant for physical applications. Apart from the treatment of an actual open chain it can also be used to approximate spin chains with a finite density of non-magnetic impurities, see [47]. Therefore, we will pay special attention to this case.

The finite temperature partition function is

\[ Z \equiv \text{Tr} \, e^{-H/T} \equiv e^{-F/T}. \]  
(2.2)

In large volume the free energy is expected to behave as

\[ F = fL + 2F_B + O(e^{-\kappa L}), \]  
(2.3)

where \( f \) is the free energy density defined as

\[ f = - \lim_{L \to \infty} \frac{T \log(Z)}{L} \]  
(2.4)

and the boundary contribution is

\[ 2F_B = - \lim_{L \to \infty} [T \log(Z) + fL]. \]  
(2.5)
We included a factor of 2 in the definition above, such that $F_B$ describes the contribution of a single boundary. The correction terms in (2.3) decay exponentially with the volume, where $1/\kappa$ is a finite temperature correlation length. Our goal is to compute $F_B$ in terms of the temperature and the boundary magnetic fields.

The Hamiltonian (2.1) is integrable for any values of the boundary magnetic fields. This can be seen by embedding it into a family of commuting boundary transfer matrices [4], which we briefly summarize below.

For the construction we will use the trigonometric $R$-matrix [53] with the normalization

$$R(u) = \begin{pmatrix}
\sinh(u + \eta) & 0 & 0 & 0 \\
0 & \sinh(u) & \sinh(\eta) & 0 \\
0 & \sinh(\eta) & \sinh(u) & 0 \\
0 & 0 & 0 & \sinh(u + \eta)
\end{pmatrix}. \quad (2.6)$$

Here the parameter $\eta$ is related to the anisotropy as $\Delta = \cosh(\eta)$; this is derived below when we relate the Hamiltonian (2.1) to the transfer matrices. In the so-called massive regime with $\Delta > 1$ we have $\eta \in \mathbb{R}^+$, whereas in the massless case we will use the variable $\gamma = \cos^{-1}(\Delta)$ with $\gamma \in (0, \pi/2)$. This $R$-matrix corresponds to the statistical weights of the 6-vertex model as given in figure 1.

The $R$-matrix satisfies the Yang–Baxter equation

$$R_{1,2}(u)R_{1,3}(u + v)R_{2,3}(v) = R_{2,3}(v)R_{1,3}(u + v)R_{1,2}(u) \quad (2.7)$$

and the unitarity and crossing relations

$$R_{1,2}(u)R_{2,1}(-u) = \sinh(u + \eta) \sinh(-u + \eta) \quad (2.8)$$

$$-R_{1,2}(-u) = \sigma_1^{\gamma} R_{1,2}^\dagger(u - \eta)\sigma_1^{\gamma} = \sigma_1^{\gamma} R_{1,2}^{\dagger}(u - \eta) \sigma_1^{\gamma}. \quad (2.9)$$

Let $H = \bigotimes_{j=1}^L \mathbb{C}^2$ be the Hilbert space of the spin chain. We define two monodromy matrices acting on $H \otimes \mathbb{C}^2$ as

$$T(\lambda) = R_{a,L}(\lambda) \ldots R_{a,1}(\lambda)$$

$$\tilde{T}(\lambda) = R_{a,1}(-\lambda) \ldots R_{a,L}(-\lambda), \quad (2.10)$$

where the index $a$ refers to the auxiliary quantum space. The boundary transfer matrix is then defined as [4]

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where $K^{\pm}$ are the so-called $K$-matrices acting on $\mathbb{C}^2$. They are given as

\begin{equation}
K^-(\lambda) = K(\lambda), \quad K^+(\lambda) = K(\lambda + \eta)
\end{equation}

with $K(\lambda)$ being the solution of the boundary Yang–Baxter (BYB) equations [3, 4]

\begin{equation}
R_{1,2}(u - w)K_1(u)R_{1,2}(u + w)K_2(w) = K_2(w)R_{1,2}(u + w)K_1(u)R_{1,2}(u - w).
\end{equation}

It follows from the YB and BYB equations that for arbitrary spectral parameters

\begin{equation}
[t(u), t(w)] = 0.
\end{equation}

In the XXZ spin chain the solutions to (2.13) form a 3-parameter family [14]. We use the parametrization in terms of the variables $(\alpha, \beta, \theta)$ as

\begin{align}
K_{11}(u, \alpha, \beta, \theta) &= 2(\sinh(\alpha) \cosh(\beta) \cosh(u) + \cosh(\alpha) \sinh(\beta) \sinh(u)) \\
K_{12}(u, \alpha, \beta, \theta) &= e^\theta \sinh(2u) \\
K_{21}(u, \alpha, \beta, \theta) &= e^{-\theta} \sinh(2u) \\
K_{22}(u, \alpha, \beta, \theta) &= 2(\sinh(\alpha) \cosh(\beta) \cosh(u) - \cosh(\alpha) \sinh(\beta) \sinh(u)).
\end{align}

The $K$-matrices satisfy the boundary crossing relation [4]

\begin{equation}
K_a(u) = \frac{1}{\sinh(2(\eta - u))} \text{Tr}_b(P_{ab}R_{ab}(-2u)K_b(u - \eta)),
\end{equation}

where $P_{ab}$ is the permutation operator.

In (2.12) we chose the same solution of (2.13) for the two $K$-matrices, and we will only have one set of boundary parameters $(\alpha, \beta, \theta)$. This corresponds to having the same boundary magnetic fields at the two ends of the chain.

The Hamiltonian is related to the first derivative of the transfer matrix at a specific rapidity value. Although it is a textbook exercise to establish this relation, we perform it here in detail, in order to fix all additive constants in the Hamiltonian.

The $R$-matrix satisfies $R(0) = \sinh(\eta)P$ and $K^{-}(0)$ is proportional to the identity, therefore

\begin{equation}
t(0) = \frac{\sinh^{2L}(\eta)\text{Tr}(K^{+(0)})\text{Tr}(K^{-}(0))}{2} \times 1.
\end{equation}

For the derivative evaluated at $u = 0$ we get

\begin{equation}
\dot{t}(0) = \sinh^{2L}(\eta) \left(\text{Tr}(K^{+(0)})\dot{K}_1^{-}(0) + \text{Tr}(\dot{K}^{+(0)})K_1^{-}(0)\right)
+ \sinh^{2L-1}(\eta) \left[\sum_{j=1}^{L-1}h_{j,j+1}\text{Tr}(K^{+(0)})K_1^{-}(0) + \text{Tr}(K_0^{+(0)}h_{0,L})K_1^{-}(0)\right],
\end{equation}

where we defined

\begin{equation}
h_{a,b} = 2P_{a,b}\dot{R}_{a,b}(0) = \sigma^+_a\sigma^-_b + \sigma^+_b\sigma^-_a + \Delta(\sigma^+_a\sigma^-_b + 1).
\end{equation}

This leads to the relation

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\[ t^{-1}(0)i(0) = \frac{1}{\sinh(\eta)} H_B, \]  

(2.20)

where \( H_B \) is a Hamiltonian operator given by

\[ H_B = \sinh(\eta) \left( \frac{\hat{K}_1^{-}(0)}{\hat{K}_1(0)} + \frac{\text{Tr}(\hat{K}(0))}{\text{Tr}(\hat{K}^{-}(0))} \right) + \frac{\text{Tr}(\hat{K}_0^{-}(0)h_{0,L})}{\text{Tr}(\hat{K}^{-}(0))} + \sum_{j=1}^{L-1} h_{j,j+1}. \]  

(2.21)

It is important that \( H_B \) is not identical to (2.1); it differs in certain additive terms. Using (2.12), (2.15) and (2.19) we obtain the explicit representation

\[ H_B = \sum_{j=1}^{L-1} h_{j,j+1} + \sum_{a=x,y,z} h_a (\sigma^a_1 + \sigma^a_L) - \frac{1}{\Delta} + 2\Delta, \]  

(2.22)

with the boundary fields

\[ h_x = \frac{\sinh(\eta) \cosh(\theta)}{\sinh(\alpha) \cosh(\beta)}, \]
\[ h_y = \frac{i \sinh(\eta) \sinh(\theta)}{\sinh(\alpha) \cosh(\beta)}, \]
\[ h_z = \sinh(\eta) \coth(\alpha) \tanh(\beta). \]  

(2.23)

The parameter \( \theta \) describes the angle of the transverse magnetic fields within the \( x-y \) plane. Due to rotational symmetry we are free to set \( \theta = 0 \), which leads to \( h_y = 0 \).

In the massive regime \( \eta \in \mathbb{R} \), and real magnetic fields are obtained if \( \alpha, \beta \) are both real or if they both have imaginary parts equal to \( \pm i\pi/2 \). The latter case corresponds to an exchange of the roles of the two parameters, and for simplicity we require that \( \alpha, \beta \in \mathbb{R} \). The case of purely longitudinal fields is reached by sending one of the parameters to infinity:

\[ h_z = \begin{cases} \sinh(\eta) \coth(\alpha) & \text{if } \beta \to \infty \\ \sinh(\eta) \tanh(\beta) & \text{if } \alpha \to \infty. \end{cases} \]  

(2.24)

Choosing the cases according to the magnitude of \( h_z \) the full range can be covered with \( \alpha, \beta \in \mathbb{R} \).

In the massless regime \( \eta = i\gamma \) with \( \gamma \in \mathbb{R} \), and all real magnetic fields can be produced by \( \alpha = i\tilde{\alpha} \) and \( \tilde{\alpha}, \beta \in \mathbb{R} \). Longitudinal fields are reached when \( \beta \to \infty \) such that

\[ h_z = \sin(\gamma) \cot(\tilde{\alpha}). \]  

(2.25)

Free boundary conditions are obtained further by setting \( \tilde{\alpha} = \pi/2 \).

For practical purposes we also present the inversion of the relations (2.23) (with \( h_y = 0 \)):

\[ \alpha = \frac{1}{2} \left[ \sinh^{-1} \left( \frac{\sinh(\eta) + h_z}{h_x} \right) + \sinh^{-1} \left( \frac{\sinh(\eta) - h_z}{h_x} \right) \right], \]
\[ \beta = \frac{1}{2} \left[ \sinh^{-1} \left( \frac{\sinh(\eta) + h_z}{h_x} \right) - \sinh^{-1} \left( \frac{\sinh(\eta) - h_z}{h_x} \right) \right]. \]  

(2.26)
These relations are valid in both regimes and they produce the $\alpha, \beta$ in accordance with the previous discussion.

In (2.22) the two boundary terms are exactly equal, even though they originate from formally different expressions in (2.21). This is not a coincidence: their agreement can be proven from the crossing relation (2.16), as it was originally remarked by Sklyanin [4].

The differences in the additive terms in $H$ and $H_B$ originate from the overall normalization of the $R$-matrix and the $K$-matrices. In the intermediate calculations we will work with $H_B$, because certain expressions are simpler this way. The original Hamiltonian is then restored through the relation

$$H = H_B - 2\Delta L + \frac{1}{\Delta}.$$  

(2.27)

This intermediate relation is singular for the specific $\Delta \to 0$ limit, but our final formulas for the boundary free energy (with respect to $H$) have a finite $\Delta \to 0$ limit.

2.2. The TBA approach

A natural way to evaluate thermal partition functions in integrability is to express them as a sum over all eigenstates of the system, to derive the Bethe equations characterizing the spectrum, and to perform a saddle point approximation of the summation to obtain the free energy. This method is known as the thermodynamic Bethe ansatz (TBA) [26, 30]. Originally devised to compute the free energy density, the TBA is also capable to capture all $\mathcal{O}(1)$ contributions to the free energy: it was shown in [40, 41], that the resulting finite terms include simple integrals (that arise from rapidity shifts of the bulk particles due to the boundaries) and two boundary-independent Fredholm determinants, which result from the fluctuations around the saddle point solution of the TBA, and the non-trivial density of states in rapidity space. The papers [40, 41] provided very general results, and in principle they could be applied to the XXZ spin chain as well. However, there are two difficulties associated with this approach.

First of all, the Bethe ansatz equations of the boundary spin chain do not always take the usual product form that was assumed in [40, 41]. In fact, for generic boundary parameters one has to deal with inhomogeneous T-Q equations and polynomial equations describing the spectrum [8, 17–22]. In principle this difficulty could be avoided by concentrating on those special cases [9, 15, 16] where the inhomogeneous terms vanish and the usual Bethe ansatz equations are recovered. In the thermodynamic limit these special points become dense in the space of boundary conditions, and by continuity they would give the boundary free energy for arbitrary magnetic fields [9].

A second difficulty with the TBA approach is that the resulting Fredholm determinants reflect the particle content of the theory, and they act in the direct sum of the rapidity spaces of all the particles. The XXZ spin chain typically has an infinite number of string solutions, and in the TBA they are treated as independent particles. This would lead to infinite dimensional Fredholm determinants.$^3$

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$^3$ These Fredholm determinants were actually presented in [52], although in a different context, see section 2.5 there.
We believe that the TBA would lead to correct final results, but their numerical implementation would be demanding. In the present work we take a different approach. We compute the boundary free energy using the quantum transfer matrix method, and show that this leads to single integrals and one dimensional Fredholm determinants. In the Conclusions we give a few additional remarks about the relation between the two approaches.

The QTM method does not require the knowledge of the spectrum of the original Hamiltonian (2.1), therefore we do not review its solution. We refer the interested reader to the papers cited above.

2.3. The QTM approach

Following [48] we develop a lattice path integral for the partition function (2.2), and we evaluate it in the large volume limit. The key idea is to build an alternative transfer matrix (called the QTM) which acts along the space direction of the corresponding 2D statistical physical system [31]. This is completely analogous with the usual step of exchanging the space and time directions in integrable (euclidean) QFT [27, 39].

It follows from (2.20) that exponentials of $\tilde{H}_B$ can be evaluated in the so-called Trotter expansion as

$$\text{Tr} \ e^{-H_B/T} = \lim_{N \to \infty} \text{Tr} \left( 1 - \frac{H_B}{TN} \right)^N = \lim_{N \to \infty} t^{-N(0)}\tilde{Z}(N, L),$$

(2.28)

where we defined

$$\tilde{Z}(N, L) = \text{Tr} \ t^{N(-\omega)}.$$

(2.29)

Here $N$ is called the Trotter number, and $\omega$ is an $N$-dependent parameter given by

$$\omega = \frac{\sinh \eta}{NT}.$$  

(2.30)

Certain intermediate formulas in the following sections can depend on the parity of $N$. For simplicity we will assume that $N$ is even.

Comparing to (2.27) we find that

$$Z = e^{-F/T} = e^{-\frac{1}{2\pi} + \frac{i2\pi L}{2\pi}} \lim_{N \to \infty} \left[ t^{-N(0)}\tilde{Z}(N, L) \right].$$  

(2.31)

With the repeated use of (2.9) one gets

$$\tilde{T}(-u) = \sigma_y^\eta T^{i\eta}(-u - \eta)\sigma_y^\eta.$$  

(2.32)

It follows that $\tilde{Z}(N, L)$ is equal to the partition function of the six vertex model with boundaries and spectral parameters as specified in the figure 2, where the vertices are given by the $R$-matrix (2.6) and the boundary weights follow from the $K$-matrices; explicit formulas will be given below.

The main idea to evaluate this partition function in the large volume limit is to build a transfer matrix that acts in the horizontal direction. This operator is called the quantum transfer matrix [31, 54]. It can be established algebraically by a reordering of the $R$-matrices under the trace in (2.29) (for a detailed computation relevant
to the present problem see \cite{49}). Alternatively, it can be constructed by performing a reflection of the partition function of figure 2 around the North–East axis, and by building a new transfer matrix that acts in the vertical direction, but acting on a spin chain with alternating inhomogeneities. This leads to the construction of the ‘quantum monodromy matrix’ as
\[
T_{QTM}(u) = R_{2N,0}(u - \eta + \omega)R_{2N-1,0}(u - \omega) \ldots R_{2,0}(u - \eta + \omega)R_{1,0}(u - \omega),
\]
where \(\omega\) is the parameter defined in (2.30). The quantum transfer matrix is then given by
\[
t_{QTM}(u) = \text{Tr} \, T_{QTM}(u).
\]
It can be read off figure 2 that the partition function can be evaluated as
\[
\bar{Z}(N, L) = \langle \Psi_+(\omega) | t_{QTM}^L(0) | \Psi_-(\omega) \rangle,
\]
where \(\langle \Psi_+(\omega) \rangle\) and \(| \Psi_-(\omega) \rangle\) are initial and final states given by the boundary conditions. They are tensor product of two site blocks:
\[
| \Psi_-(\omega) \rangle = \otimes_{j=1}^N | \psi_-(\omega) \rangle \quad \langle \Psi_+(\omega) \rangle = \otimes_{j=1}^N \langle \psi_+(\omega) |,
\]
where the local two-site states are defined as
\[
| \psi_-(\omega) \rangle = \sum_{j_1,j_2=1}^2 \psi_-(\omega, j_1, j_2) \, | j_2 \rangle_2 \otimes | j_1 \rangle_1
\]
\[
\langle \psi_+(\omega) | = \sum_{j_1,j_2=1}^2 \langle \psi_+(\omega, j_1, j_2) \, | j_2 \rangle_2 \otimes | j_1 \rangle_1.
\]
The components can be read off (2.11)–(2.32):
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\[ \psi_-(\omega, j_1, j_2) = (\sigma^y K_-(\omega))^{j_2}_{j_1} \quad \psi_+(\omega, j_1, j_2) = (K_+(-\omega)\sigma^y)^{j_1}_{j_2}. \]  

(2.38)

Here the convention is such that the index \( j_1 \) refers to the lower lines in figure 2.

It is important that the two boundary states are not identical to each other, because the \( K \)-matrices are evaluated at different rapidity parameters. The crossing relation (2.16) relates the two boundary states to each other, however, this will not be used explicitly. We also remark that the boundary states are not normalized to unity. In fact we have

\[ \langle \tilde{\Psi}_j | \Psi_{\omega}(\omega) \rangle = \frac{\text{Tr} (K_-(-\omega)K_+(\omega))}{\text{Tr}(K^+(0))\text{Tr}(K^-(0))} \]

(2.39)

Let \( \langle \tilde{\Psi}_j | \text{and} | \Psi_j \rangle \) denote the left- and right-eigenvectors of \( T_{\text{QTM}}(u) \), with the normalization

\[ \langle \tilde{\Psi}_j | \Psi_k \rangle = \delta_{jk}. \]

(2.40)

The quantum transfer matrix is not hermitian, therefore the two sets of vectors are not hermitian conjugates of each other. They can be related to each other by a crossing transformation, but this will not be used here.

Using the complete set of states the partition function (2.35) is evaluated as

\[ Z(N, L) = \sum_j \Lambda_j^N \langle \Psi_+|\omega)\langle\Psi_j|\Psi_-(\omega)\rangle \]

(2.41)

where \( \Lambda_j \) are the eigenvalues of the QTM for the special rapidity \( u = 0 \). It is known that there is a finite gap in the set of the eigenvalues even in the \( N \to \infty \) limit \([54]\). Therefore, in the large volume limit it is enough to keep the leading eigenvector with the maximal eigenvalue. This state will be denoted by \( |\Psi_0\rangle \), with the eigenvalue being \( \Lambda_0 \).

Using the relation (2.31) we get

\[ e^{-F/T} = e^{-\frac{\Delta}{T} + \frac{2\Delta L}{T}} \lim_{N \to \infty} \left[ \frac{2N \sinh^{-2L N}(\eta)\Lambda_0^N \langle \Psi_+|\omega)\langle\Psi_0|\Psi_-(\omega)\rangle}{\text{Tr}(K^+(0))\text{Tr}(K^-(0))} \right] + O(e^{-\kappa L}), \]

(2.42)

where \( \kappa \) is the gap in the eigenvalues in the Trotter limit.

Isolating the \( O(L) \) and \( O(1) \) terms we get

\[ e^{-f/T} = e^{2\Delta/T} \lim_{N \to \infty} \frac{\Lambda_0}{\sinh^{2N}(\eta)} , \]

(2.43)

and for the boundary free energy

\[ e^{-2F_B/T} = e^{-\frac{\Delta}{T} \lim_{N \to \infty} \left[ \frac{2}{\text{Tr}(K^+(0))\text{Tr}(K^-(0))} \right]^N \langle \Psi_+|\omega)\langle\Psi_0|\Psi_-(\omega)\rangle} . \]

(2.44)

2.4. Bethe ansatz for the QTM

In order to compute (2.44) we need a description of the dominant eigenvector of the QTM. This can be given by the algebraic Bethe ansatz (ABA), which will be summarized below. For a more detailed exposition we refer the reader to \([54, 55]\). It
is important that the diagonalization of the QTM is completely independent of the boundary conditions of the physical spin chain, and it is always done by the standard techniques of ABA that apply to a periodic (inhomogeneous) spin chain.

We write the monodromy matrix in auxiliary space as the block-matrix

$$T_{\text{QTM}}(u) = \begin{pmatrix} A(u) & B(u) \\ C(u) & D(u) \end{pmatrix}. \quad (2.45)$$

Right eigenstates of the transfer matrix can be constructed as

$$|\Psi\rangle \sim \prod_{k=1}^{n} B(\lambda_k)|0\rangle. \quad (2.46)$$

Here $|0\rangle$ is the reference state with all spins up, and the $\lambda_k$ are the Bethe rapidities. The reference state is annihilated by the $C$-operators and it is an eigenvector of $A$ and $D$ with the eigenvalues

$$a(u) = (\sinh(u + \omega) \sinh(u - \omega + \eta))^N \quad d(u) = (\sinh(u - \omega) \sinh(u + \omega - \eta))^N.$$

A state (2.46) is an eigenstate if it satisfies the Bethe equations

$$a(\lambda_j) + 1 = 0, \quad j = 1 \ldots n, \quad (2.47)$$

where we defined the auxiliary function as

$$a(\lambda) = d(\lambda) \frac{\prod_{k=1}^{n} \sinh(\lambda - \lambda_k + \eta)}{\prod_{k=1}^{n} \sinh(\lambda - \lambda_k - \eta)} = \left( \frac{\sinh(\lambda - \eta + \omega) \sinh(\lambda - \omega)}{\sinh(\lambda + \eta - \omega) \sinh(\lambda + \omega)} \right)^N \prod_{k=1}^{n} \frac{\sinh(\lambda - \lambda_k + \eta)}{\sinh(\lambda - \lambda_k - \eta)}. \quad (2.48)$$

As we will see below, the function $a(u)$ has a finite Trotter limit for the ground state of the QTM. In the formulas below we will use the same notation $a(u)$ for finite $N$ and also for $N \to \infty$.

The corresponding eigenvalue of the transfer matrix is

$$\Lambda(u) = a(u) \prod_{j=1}^{n} \frac{\sinh(\lambda_j - u + \eta)}{\sinh(\lambda_j - u)} + d(u) \prod_{j=1}^{n} \frac{\sinh(\lambda_j - u - \eta)}{\sinh(\lambda_j - u)}. \quad (2.49)$$

At the special rapidity $u = 0$ this gives

$$\Lambda(0) = (\sinh(\omega) \sinh(\eta - \omega))^N \left( \prod_{j=1}^{n} \frac{\sinh(\lambda_j + \eta)}{\sinh(\lambda_j)} + \prod_{j=1}^{n} \frac{\sinh(\lambda_j - \eta)}{\sinh(\lambda_j)} \right). \quad (2.50)$$

Similar to (2.46), left-eigenvectors can be constructed as

$$\langle \Psi| \sim \langle 0| \prod_{k=1}^{n} C(\lambda_k). \quad (2.51)$$

The normalization factors associated to these vectors are [56]
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\[
\langle 0 \rangle \prod_{k=1}^{n} C(\lambda_k) \prod_{k=1}^{n} B(\lambda_k) | 0 \rangle = \sinh^n(\eta) \prod_{j=1}^{n} (\alpha(\lambda_j) d(\lambda_j)) \prod_{j \neq k} \left( f(\lambda_j, \lambda_k) \times \det G^{[n]} \right),
\]

where

\[
f(\lambda, \mu) = \frac{\sinh(\lambda - \mu + \eta)}{\sinh(\lambda - \mu)}
\]

and \( G^{[n]} \) is the so-called Gaudin matrix given by

\[
G_{jk}^{[n]} = \delta_{jk} m_j - \varphi(\lambda_j - \lambda_k)
\]

with

\[
m_j = \frac{\alpha'(\lambda_j)}{\alpha(\lambda_j)}
\]

and

\[
\varphi(\lambda) = -\frac{\sinh(2\eta)}{\sinh(\lambda + \eta) \sinh(\lambda - \eta)}.
\]

It is known that the leading eigenvector of the QTM has \( n = N \) rapidities which come in pairs and can be denoted as

\[
\{ \lambda \}_N = \{ \lambda^+, -\lambda^+ \}_{N/2} = \{ \lambda^+_1, -\lambda^+_1, \lambda^+_2, -\lambda^+_2, \ldots, \lambda^+_N, -\lambda^+_N \}.
\]

This holds for arbitrary temperatures. In the massive regime all \( \lambda^+ \) are purely imaginary, whereas for \( \Delta < 1 \) they are real. For a more detailed discussion of the Bethe roots of the QTM we refer the reader to \([54]\).

The advantage of the auxiliary function is that sums over the Bethe roots can be expressed as contour integrals involving \( \alpha(u) \), and that \( \alpha(u) \) has a finite \( N \to \infty \) limit. Moreover, there are simple non-linear integral equations (NLIE’s) that determine \( \alpha(u) \) both at finite \( N \) and in the Trotter limit. In the remainder of this section we repeat the main steps in deriving these NLIE’s. Essentially the same steps will be used later to derive the integral representations for the boundary free energy.

First we note that both \( \alpha(u) \) and \( \Lambda(u) \) are periodic in the imaginary direction with period \( i\pi \). Second, we define the so-called physical strip. In the massive case this consists of the points of complex plane with \(|\Re(z)| < \eta/2, |\Im(z)| < \pi/2\), whereas in the massless case we require \(|\Im(z)| < \gamma/2\). The most important property of the physical strip is that the only zeroes of \( 1 + \alpha(u) \) within the strip are the Bethe roots, and this is why we can use the contour integral techniques for the sums over Bethe roots \([54]\).

As customary we define a contour \( C \) such that it encircles all Bethe roots and the \( N \)-order pole of \( \alpha(\lambda) \) at \( \lambda = -\omega \), but it does not include additional poles or zeroes of \( 1 + \alpha(\lambda) \) \([54]\). As remarked above, this means that \( C \) has to stay in the physical strip. In the massive regime the contour can be chosen as the union of two vertical segments \([-i\pi/2 + a \ldots i\pi/2 + a]\) and \([-i\pi/2 - a \ldots i\pi/2 - a]\) with \( a < \eta/2 \). In the massless regime the usual choice is the union of \( \mathbb{R} + ia \) and \( \mathbb{R} - ia \) with \( a < \gamma/2 \), but for our present purposes it is important to choose a compact contour. One possibility is to choose an ellipse whose axes coincide with the real and imaginary axis, such that the minor axis

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is smaller than $\gamma/2$ and the major axis is large enough to include all Bethe roots; this is our choice for the numerical investigations, to be presented in section 9.

As a first step we express the logarithm of $a(\lambda)$ as

$$
\log a(\lambda) = N \log \left( \frac{\sinh(\lambda + \eta + \omega) \sinh(\lambda - \omega)}{\sinh(\lambda + \eta - \omega) \sinh(\lambda + \omega)} \right) - N \frac{\sinh(\lambda + \eta + \omega)}{\sinh(\lambda - \omega)} + \sum_{k=1}^{N} \log \frac{\sinh(\lambda - \lambda_k + \eta)}{\sinh(\lambda - \lambda_k - \eta)}.
$$

(2.58)

Within the contour $C$ the function $1 + a(u)$ has an $N$-fold pole at $u = -\omega$ and $N$ zeroes at the Bethe roots. Therefore $\log(1 + a(u))$ can be defined as a single valued function on the contour. Let us choose a function $f$ that does not have poles or zeros within the contour. Then from integration by parts we get the formula

$$
\log \left( \prod_{n=1}^{N} f(\lambda_n) \right) = - \oint_{C} \frac{dv}{2\pi i} f'(v) \log (1 + a(v)) + N \log f(-\omega).
$$

(2.59)

Applying this identity with $f(v) = \frac{\sinh(v+\lambda+\eta)}{\sinh(v-\lambda-\eta)}$ we get

$$
\log a(\lambda) = N \log \left( \frac{\sinh(\lambda + \eta + \omega) \sinh(\lambda - \omega)}{\sinh(\lambda + \eta - \omega) \sinh(\lambda + \omega)} \right) + \int_{C} \frac{dv}{2\pi} \varphi(\lambda - \nu) \log(1 + a(\nu)).
$$

(2.60)

This integral equation is valid at any finite Trotter number $N$ and for any parameter $\omega$. Also, it has a finite Trotter limit given by

$$
\log a(\lambda) = - \frac{1}{T} \frac{2 \sinh^2(\eta)}{\sinh(\lambda) \sinh(\lambda + \eta)} + \int_{C} \frac{dv}{2\pi} \varphi(\lambda - \nu) \log(1 + a(\nu)).
$$

(2.61)

The transfer matrix eigenvalue is determined similarly. From (2.49) we have

$$
\log \Lambda(u) = \log(1 + a(u)) + N \log((\sinh(u + \omega) \sinh(u - \omega + \eta))) + \sum_{j=1}^{N} \frac{\sinh(\lambda_j - \eta)}{\sinh(\lambda_j - u)}.
$$

(2.62)

Applying (2.59) with $f(v) = \frac{\sinh(v+\lambda+\eta)}{\sinh(v-\lambda-\eta)}$ with $u$ outside the contour we get

$$
\log \Lambda(u) = \log(1 + a(u)) + N \log((\sinh(\omega + \eta) \sinh(u - \omega + \eta)))
$$

$$
+ \int_{C} \frac{dv}{2\pi} \frac{\sinh(\eta)}{\sinh(\nu + \eta) \sinh(\nu - u)} \log(1 + a(\nu)).
$$

(2.63)

We can analytically continue this formula to the case when $u$ is inside the contour. In this case we pick up a pole contribution and (using also that $N$ is even)

$$
\log \Lambda(u) = N \log((\sinh(-\omega + \eta) \sinh(-\omega + \eta)))
$$

$$
+ \int_{C} \frac{dv}{2\pi} \frac{\sinh(\eta)}{\sinh(\nu + \eta) \sinh(\nu - u)} \log(1 + a(\nu)).
$$

(2.64)

Specifically for $u = 0$

$$
\log \Lambda(0) = 2N \log((\sinh(\omega + \eta))) + \int_{C} \frac{dv}{2\pi} \frac{\sinh(\eta)}{\sinh(\nu + \eta) \sinh(\nu)} \log(1 + a(\nu)).
$$

(2.65)
Thus for the free energy density we get from (2.43)

\[
\frac{f}{T} = -2\Delta/T - \lim_{N \to \infty} \frac{2N \log \sinh(\omega + \eta)}{\sinh(\eta)} - \oint_{C} \frac{d\nu}{2\pi i} \frac{\sinh(\eta)}{\sinh(\nu + \eta) \sinh(\nu)} \log (1 + a(\nu)) = -\oint_{C} \frac{d\nu}{2\pi i} \frac{\sinh(\eta)}{\sinh(\nu + \eta) \sinh(\nu)} \log (1 + a(\nu)).
\]

(2.66)

In the calculation of the boundary free energy the special rapidity \(i\pi/2\) will be of importance. From the definition (2.48) it can be seen that \(a(i\pi/2) = 1\) for any \(\omega\) and \(N\). This value is thus constant even in the Trotter limit, for any temperature.

3. Scalar products

In this section we treat the scalar products between the eigenstates of the QTM and the boundary states. Our goal is to find convenient determinant formulas for the products

\[
\langle \Psi_+(\omega) | \Psi \rangle \langle \tilde{\Psi} | \Psi_-(\omega) \rangle,
\]

(3.1)

which enter formula (2.44). We stress that the Bethe states are normalized to unity, but the boundary states have a non-trivial norm given by (2.39). According to the previous section, such products can be evaluated in the algebraic Bethe ansatz as

\[
\frac{\langle \Psi_+(\omega) | \prod_{k=1}^{n} B(\lambda_k) | 0 \rangle \langle 0 | \prod_{k=1}^{n} C(\lambda_k) | \Psi_-(\omega) \rangle}{\langle 0 | \prod_{k=1}^{n} C(\lambda_k) \prod_{k=1}^{n} B(\lambda_k) | 0 \rangle}.
\]

(3.2)

The un-normalized overlaps in the numerator are related to each other as

\[
\langle \Psi_+(\omega) | \prod_{k=1}^{n} B(\lambda_k) | 0 \rangle = \left( \frac{\sinh(2(\eta - \omega))}{\sinh(2\omega)} \right)^n \langle 0 | \prod_{k=1}^{n} C(\lambda_k) | \Psi_-(\omega) \rangle.
\]

(3.3)

This relation was already given in [49], and it can be proven using the crossing relations (2.9) and (2.16).

Scalar products of this form were first studied in [57], where it was shown that they are related to a certain partition function of the six-vertex model with a reflecting end. In the case of diagonal \(K\)-matrices the partition function was computed by Tsushiya in [58], the resulting determinant formula is known as the Tsushiya-determinant. An alternative determinant formula for the overlaps was given in [49]. This was used as a starting point in the works [50, 51] that considered the overlaps in the homogeneous, physical spin chain. In these works it was shown that the only non-vanishing overlaps are those with states that display the pair structure, and that in these cases the scalar products can be expressed by two Gaudin-like determinants multiplied by a product of one-particle overlap functions. The formulas of [50, 51] proved to be central for the analysis of quantum quench problems in the spin chain [59–61].

The recent work [52] extended the results of [50, 51] to boundary states with non-diagonal \(K\)-matrices. It was found that the overlaps have the same structure even in this case: they involve the same Gaudin-like determinants, and only the pre-factors...
need to be modified. It was argued in [52] that the pre-factors can be fixed by a combination of the QTM and quench action methods, but the presence of the same determinants was only conjectured and numerically checked; a proof is yet missing.

In [62] it was shown by a very general, model-independent calculation that the overlaps with boundary state created by integrable \( K \)-matrices are non-vanishing only for Bethe states with the pair structure. This proof did not rely on knowledge of the exact overlaps, instead it only used the boundary Yang–Baxter relation (2.13). Therefore it also applies to the non-diagonal \( K \)-matrices.

The works [50–52, 57, 62] studied the homogeneous chain which corresponds to \( \omega = \eta/2 \) in (2.33). Fewer results are available for the inhomogeneous case, which can nevertheless be studied with the same methods. For example it can be seen easily that the proof of [62] for the pair structure holds for general \( \omega \). Moreover, the methods of [52] can be modified in a straightforward way to yield a conjecture for the overlaps relevant to this work. In the following we formulate this conjecture, whereas for a detailed calculation leading up to it we refer to [52].

Denoting by \( \{\{\pm \lambda^{+}\}_{n/2}\} \) the on-shell states with the pair structure the conjecture for the overlaps reads

\[
\langle \Psi_{+}(\omega) | \{\pm \lambda^{+}\}_{n/2} \rangle \langle \{\pm \lambda^{+}\}_{n/2} | \Psi_{-}(\omega) \rangle = (\sinh(2(\eta - \omega)) \sinh(2\omega)) N \prod_{j=1}^{n/2} u(\lambda_{j}^{+}) \times \frac{\det G_{jk}^{+,[n/2]}}{\det G_{jk}^{-,[n/2]}}. \tag{3.4}
\]

Here the single particle overlap function is defined as

\[
u_{\alpha}^{\epsilon}(\lambda) = \frac{v_{\alpha}^{\epsilon}(\lambda + \kappa) v_{\alpha}^{\epsilon}(\lambda - \kappa)}{v_{\eta/2}^{\epsilon} v_{\eta/2}^{\epsilon} v_{0}^{\epsilon} v_{0}^{\epsilon}}, \tag{3.5}
\]

where we used the short-hand notation

\[
u_{\alpha}^{\epsilon}(\lambda) = \sinh(\lambda + \kappa) \sinh(\lambda - \kappa) \quad v_{\alpha}^{\epsilon}(\lambda) = \cosh(\lambda + \kappa) \cosh(\lambda - \kappa). \tag{3.6}
\]

The two Gaudin-like matrices in (3.4) are

\[
G_{jk}^{\pm,[n/2]} = \delta_{jk} m_{j} - \left[ \phi(\lambda_{j}^{+} - \lambda_{k}^{+}) \pm \phi(\lambda_{j}^{+} + \lambda_{k}^{+}) \right]. \tag{3.7}
\]

The differences between the present formula (3.4) and the main result in [52] (equation (3.13) there) are the following:

- In the present case the length of the (auxiliary) spin chain is \( 2N \), because is the overlap is calculated in the channel of the quantum transfer matrix. In [52] the length of the spin chain was denoted by \( L \), and it referred to the physical spin chain.
- Here the boundary states are not normalized; overlaps with normalized states are obtained by dividing with the factor given by (2.39).
- The Gaudin-like matrices \( G_{\pm} \) are expressed in terms of the auxiliary function: the diagonal elements \( m_{j} \) are given by (2.55). This functional form holds for any \( \omega \), including the homogeneous case. However, \( a(\lambda) \) depends explicitly on \( \omega \), thus the diagonal elements of \( G_{\pm} \) differ from those in [50–52].
Here we have a non-trivial overall normalization factor of $(\sinh(2(\eta - \omega)) \sinh(2\omega))^N$. This factor is found by evaluating the ‘quench action sum rule’, analogously to the calculation in [52]. The overlap formula also holds for $n = 0$, in which case this factor comes simply from the projection of the reference state onto the boundary states. These overlaps are obtained simply from (2.36) and (2.37) after the substitution

$$
\psi_+(-\omega)_{11} = -iK_+(-\omega)_{12} = i \sinh(2\omega)
\psi_+(-\omega)_{11} = iK_+(-\omega)_{21} = i \sinh(2(\eta - \omega)).
$$

These differences can be summarized as follows: after the replacements $2N \rightarrow L$ and $\omega \rightarrow \eta/2$ (and correcting with the norm (2.39)) the formula (3.4) reproduces the main result of [52].

The case of diagonal $K$-matrices can be obtained in the limit $\beta \rightarrow \infty$ by the scaling

$$
K_{\text{diag}}(u) = \lim_{\beta \rightarrow \infty} e^{-\beta K}(u) = \begin{pmatrix}
\sinh(\alpha + u) & 0 \\
0 & \sinh(\alpha - u)
\end{pmatrix}.
$$

It can be seen from (3.4) that in this limit the un-normalized overlaps scale as $e^{2\beta n}$, therefore, only the Bethe states with $n = N$ have a non-vanishing overlap with the boundary states created by the diagonal $K$-matrices. As remarked in [52], this is consistent with spin-$z$ conservation, because according to (2.37) the diagonal $K$-matrices describe states that lie in the zero-magnetization sector. In the diagonal case our conjecture can be proven rigorously using the methods of [50, 51], starting from the Tsushiya-determinant and its alternative representation given in [49]. In [50, 51] only the homogeneous case was treated, in order to arrive at the overlaps with the Néel state for the physical spin chain. However, each step can be repeated in a straightforward way also for the inhomogeneous transfer matrices, incorporating the relations (3.3) and (2.52). We performed this calculation and thus proved (3.4) in the diagonal case; we refrain from presenting this calculation here, because it is a mere repetition of the steps of [50, 51].

We also performed numerical checks of our conjecture in the case of general boundary parameters; we treated cases with small values of $N$ and $\Delta > 1$. The numerical procedure included the solution of the Bethe equations (2.47), which is relatively easy as all roots lie on a finite segment on the imaginary axis. The numerical predictions of (3.4) were then compared to real space calculation of the overlaps, for various values of the boundary parameters. In all cases perfect agreement was found, with a relative accuracy of at least $10^{-10}$. Examples of the numerical data are shown in table 1.

4. Boundary free energy

In this section we compute the Trotter limit of the previous formulas and derive a compact representation for the boundary free energy. We treat the leading eigenstate of the QTM, whose rapidities will be denoted as

$^4$ Here we used the fact that the algebraic Bethe ansatz only treats states with $n \leq N$. 

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Table 1. Numerical examples for the overlaps (3.4) for the leading eigenstate of the QTM, for small values of $N$. We denote $S = \langle \Psi_{\pm}(\omega)|\{\pm \lambda^+\}_{N/2}\{\pm \lambda^+\}_{N/2}|\Psi_{\pm}(\omega)\rangle$, where the left and right eigenstates are normalized to $\langle\{\pm \lambda^+\}_{N/2}\{\pm \lambda^+\}_{N/2}|1\rangle = 1$ and the boundary states are given by (2.36). In these examples we chose $\Delta = 2$ such that the rapidities are purely imaginary. We chose the arbitrary parameters $T = 1, \alpha = 0.1$ and $\beta = 1.5$. The relative error of the formula (3.4) was smaller than $10^{-10}$ in all three cases. Similar errors were observed for other values of $\Delta$ and the boundary parameters.

| $N$ | $\{\text{Im}(\lambda^+)\}_{N/2}$ | $S$ |
|-----|---------------------------------|-----|
| 2   | 0.337728                        | 63.022646 |
| 4   | 0.146496, 0.6260620             | 2773.2102 |
| 6   | 0.0711016, 0.2514235, 0.6705907 | 30066.783 |

\begin{align}
\{\lambda\}_N = \{\lambda^+, -\lambda^+\}_{N/2} = \{\lambda^+_1, -\lambda^+_1, \lambda^+_2, -\lambda^+_2, \ldots, \lambda^+_{N/2}, -\lambda^+_{N/2}\}.
\end{align}

Starting from (2.44) and (3.4), and computing the traces of the $K$-matrices as

\begin{align}
\text{Tr}(K^-(0)) = 4 \sinh(\alpha) \cosh(\beta) \quad \text{Tr}(K^+(0)) = 4 \sinh(\alpha) \cosh(\beta) \cosh(\eta)
\end{align}

we obtain

\begin{align}
e^{-2\beta F_B} = e^{-\frac{1}{\cosh(\eta) \cosh(\eta)}} \lim_{N \to \infty} \left(\frac{\cosh(\eta - \omega)}{\cosh(\eta)}\right)^N \left(\frac{\sinh(\eta - \omega)}{\sinh(\eta - 2\omega)}\right)^N \times \prod_{j=1}^{N} \left[\frac{\sinh^2(\lambda_j + \alpha) \cosh^2(\lambda_j + \beta)}{\sinh^2(\alpha) \cosh^2(\beta)} \frac{\sinh(2\omega)}{\sinh(2\lambda_j)} \frac{\sinh(\eta - 2\omega)}{\sinh(2\lambda_j + \eta)}\right] \times \frac{\det G^+_{+[N/2]}}{\det G^-_{-[N/2]}}.
\end{align}

The Trotter limit of the first two pre-factors is

\begin{align}
\lim_{N \to \infty} \left(\frac{\cosh(\eta - \omega)}{\cosh(\eta)}\right)^N \left(\frac{\sinh(\eta - \omega)}{\sinh(\eta - 2\omega)}\right)^N = e^{-\frac{1}{\cosh(\eta) \cosh(\eta)}}
\end{align}

leading to the simplified expression

\begin{align}
e^{-2\beta F_B} = \lim_{N \to \infty} \prod_{j=1}^{N} \left[\frac{\sinh^2(\lambda_j + \alpha) \cosh^2(\lambda_j + \beta)}{\sinh^2(\alpha) \cosh^2(\beta)} \frac{\sinh(2\omega)}{\sinh(2\lambda_j)} \frac{\sinh(\eta - 2\omega)}{\sinh(2\lambda_j + \eta)}\right] \times \frac{\det G^+_{+[N/2]}}{\det G^-_{-[N/2]}}.
\end{align}

The Gaudin-like matrices are convenient for a numerical analysis at finite Trotter number, but they are somewhat difficult to treat in the Trotter limit. Our goal is to express them as Fredholm determinants, therefore we rewrite them as $N \times N$ matrices. Let us define the $N \times N$ matrices $H^\pm_{jk}$ as

\begin{align}
H^\pm_{jk} = \frac{\varphi^-_{jk}}{2} \pm \frac{\varphi^+_{jk}}{2}, \quad \text{where} \quad \varphi_{jk} = \frac{\varphi(\lambda_j \pm \lambda_k)}{m_j}.
\end{align}

It can be seen from the block diagonal forms that

\begin{align}
\frac{\det G^+_{+[N/2]}}{\det G^-_{-[N/2]}} = \frac{\det (1 - H^+_{+[N]})}{\det (1 - H^-_{-[N]})},
\end{align}

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and this expression is more convenient in the subsequent calculations.

4.1. Trotter limit

We are now in the position to perform the Trotter limit. First we consider the pre-factors: we apply (2.59) to turn the products into integral expressions.

Let us consider the function \( f(u) = \sinh(u + \alpha) \) with a boundary parameter \( \alpha \) that lies outside the canonical contour. Then from (2.59) we get

\[
\log \left( \prod_{a=1}^{N} \frac{\sinh(\lambda_a + \alpha)}{\sinh(\alpha)} \right) = - \int_{C} \frac{d\nu}{2\pi i} \coth(\nu + \alpha) \log (1 + a(\nu)) + N \log \frac{\sinh(-\omega + \alpha)}{\sinh(\alpha)}. \tag{4.6}
\]

In the case when \( \alpha \) is inside the contour we have to pick up a pole contribution, leading to the general formula

\[
\log \left( \prod_{a=1}^{N} \frac{\sinh(\lambda_a + \alpha)}{\sinh(\alpha)} \right) = \delta_{\alpha} \log(1 + a(-\alpha)) \nonumber \\
- \int_{C} \frac{d\nu}{2\pi i} \coth(\nu + \alpha) \log (1 + a(\nu)) + N \log \frac{\sinh(-\omega + \alpha)}{\sinh(\alpha)}, \tag{4.7}
\]

where we used the notation that for any \( \xi \in \mathbb{C} \) we have \( \delta_{\xi} = 1 \) if \( \xi \) is inside the contour, and \( \delta_{\xi} = 0 \) otherwise.

In the Trotter limit this leads to

\[
\lim_{N \to \infty} \log \left( \prod_{a=1}^{N} \frac{\sinh(\lambda_a + \alpha)}{\sinh(\alpha)} \right) = \delta_{\alpha} \log(1 + a(-\alpha)) \nonumber \\
- \int_{C} \frac{d\nu}{2\pi i} \coth(\nu + \alpha) \log (1 + a(\nu)) - \frac{\coth(\alpha) \sinh(\eta)}{T}, \tag{4.8}
\]

Similarly

\[
\lim_{N \to \infty} \log \left( \prod_{a=1}^{N} \frac{\cosh(\lambda_a + \beta)}{\cosh(\beta)} \right) = \delta_{\beta-i\pi/2} \log(1 + a(-\beta - i\pi/2)) \nonumber \\
- \int_{C} \frac{d\nu}{2\pi i} \tanh(\nu + \beta) \log (1 + a(\nu)) - \frac{\tanh(\beta) \sinh(\eta)}{T}. \tag{4.9}
\]

By analogous calculations for the remaining two products we obtain

\[
\lim_{N \to \infty} \log \prod_{a=1}^{N} \frac{\sinh(2\omega)}{\sinh(2\lambda_j) \sinh(2\lambda_j + \eta)} = - \log(2)(1 + \delta_{\pi/2}) + \int_{C} \frac{d\nu}{2\pi i} 2(\coth(2\nu + \coth(2\nu + \xi)) \log (1 + a(\nu)). \tag{4.10}
\]

Here we used that at finite Trotter number we have the special values \( a(0) = a(i\pi/2) = 1 \). In the massive case \( \delta_{\pi/2} = 1 \), whereas in the massless case \( \delta_{\pi/2} = 0 \), therefore we will use the notation \( \delta_{\Delta > 1} \equiv \delta_{\pi/2} \).

We now evaluate the Trotter limit of the determinants. For any matrix of the form
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\[ M_{jk}^{[N]} = \delta_{jk} - \frac{a'(\lambda_j)}{a'(\lambda_j)} f(\lambda_j, \lambda_k) \] (4.11)

its determinant in the Trotter limit becomes the Fredholm determinant

\[ \lim_{N \to \infty} M_{jk}^{[N]} = \det \left( 1 - f \right), \] (4.12)

where \( f \) is an integral operator that acts as

\[ \left( f(g) \right)(x) = \int C \frac{du}{2\pi i} \frac{a(u)}{1 + a(u)} f(x, u) g(u). \] (4.13)

This can be applied to the matrices above, so that

\[ \lim_{N \to \infty} \det \left( 1 - H^{+, [N]} \right) = \det \left( 1 - \hat{H}^+ \right) \] (4.14)

where \( \hat{H}^{\pm} \) are integral operators that act as

\[ \left( \hat{H}^\pm(g) \right)(x) = \int C \frac{du}{2\pi i} \frac{\varphi(x - u) \pm \varphi(x + u)}{2} g(u). \] (4.15)

In establishing the relation (4.12) it is essential that the only zeros of \( 1 + a(u) \) inside the contour are the Bethe roots.

Putting everything together we obtain the final formula for the boundary free energy

\[ F_B/T = \frac{1 + \delta_{\Delta \geq 1}}{2} \log(2) - \delta_{-\alpha} \log(1 + a(-\alpha)) - \delta_{-\beta - i\pi/2} \log(1 + a(-\beta - i\pi/2)) \]

\[ - \int C \frac{d\nu}{2\pi i} \left[ \coth(2\nu) + \coth(2\nu + \eta) - \coth(\nu + \alpha) \right] \log(1 + a(\nu)) \]

\[ - \frac{1}{2} \log \frac{\det \left( 1 - \hat{H}^+ \right)}{\det \left( 1 - \hat{H}^- \right)} + \frac{\left( \coth(\alpha) + \tanh(\beta) \right) \sinh(\eta)}{T}. \] (4.16)

An interesting alternative formula can be derived if we express the ratio of the two determinants at finite Trotter number as

\[ \log \frac{\det \left( 1 - H^{+, [N]} \right)}{\det \left( 1 - H^{-, [N]} \right)} = - \sum_{n=1}^{\infty} \frac{1}{n} \text{Tr} \left( (H^{+, [N]})^n - (H^{-, [N]})^n \right). \] (4.17)

Using the definition of the \( H^{\pm, [N]} \) and the symmetry of the Bethe roots this is equivalent to

\[ - \sum_{n=1}^{\infty} \frac{1}{n} \text{Tr} \left( (\varphi^{-, [N]})^{n-1} \varphi^{+, [N]} \right), \] (4.18)

which can be expressed as the integral series

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The rhs has a finite Trotter limit, which can be substituted into (4.16).

Quite interestingly this expression has the same form as the boundary-independent part of the $g$-function in the TBA framework \[39–41, 63\], apart from an overall sign. This difference in the overall sign was already noticed in \[52\], although in a different context (see section 2.5 there).

The physical interpretation of the terms proportional to $\delta_{-\alpha}$ and $\delta_{-\beta-i\pi/2}$ is not evident from the finite $T$ formulas. First of all, the inclusion of these terms clearly depends on the contour itself: even if $\alpha$ and/or $\beta$ lie within the physical strip, the contours could be modified such that these terms can be avoided. Their physical meaning shows up in the $T \to 0$ limit, where they describe the contribution of boundary bound states to the ground state energy. Therefore we interpret them at finite $T$ as the contribution of the boundary bound states to the free energy. Although the $T \to 0$ limit will be investigated separately in section 6, we give here a few more comments about this issue.

In the present paper we did not discuss the solution of the Hamiltonian itself. Nevertheless it is known that the open spin chain can have bound states localized around the boundaries, and these states are represented by special Bethe roots. The bound states exist when the boundary parameters are within the physical strip \[12, 13\]. These bound states modify the energy of the Bethe states through their bare energy and also by shifting the roots of the bulk particles. Thus we can expect that they give some finite contributions to the free energy as well. We also expect that if a correct TBA result for $F_B$ were given, then these terms would show up as the result of the existence of the boundary bound states.

4.2. Special cases

Here we investigate special cases of the boundary parameters.

The case of longitudinal fields can be reached by sending one of the boundary parameters to infinity. This is most easily performed on the intermediate expression (4.4): the pair structure of the Bethe roots implies that in the $\alpha, \beta \to \infty$ limit the corresponding factors disappear from the product. Nevertheless it is also possible to perform this limit on the final formulas. For example in the $\beta \to +\infty$ limit the $\beta$-dependent terms of (4.16) become

$$\int_C \frac{d\nu}{2\pi i} \log(1 + a(\nu)) + \frac{\sinh(\eta)}{T}. \quad (4.20)$$

The integral can be symmetrized with a $\nu \to -\nu$ transformation, and by using $a(-\nu) = 1/a(\nu)$ we get

$$\int_C \frac{d\nu}{2\pi i} \log(1 + a(\nu)) = \frac{1}{2} \int_C \frac{d\nu}{2\pi i} \log \frac{1 + a(\nu)}{1 + a^{-1}(\nu)} = \frac{1}{2} \int_C \frac{d\nu}{2\pi i} \log a(\nu). \quad (4.21)$$
Using the NLIE (2.61) this is can be evaluated by contour integrals. The integral over
the convolution term gives zero, whereas
\[
\frac{1}{2} \oint_C \frac{d\nu}{2\pi i} \log a(\nu) = \frac{1}{2} \oint_C \frac{d\nu}{2\pi i} - \frac{1}{T} \frac{2\sinh^2(\eta)}{\sinh(\lambda) \sinh(\lambda + \eta)} = - \frac{\sinh(\eta)}{T}.
\] (4.22)

Altogether this shows that the sum (4.20) vanishes and for the boundary free energy
we get
\[
\frac{F_B}{T} = \frac{1}{2} \frac{\Delta_{>1}}{2} \log(2) - \delta_{-\alpha} \log(1 + a(-\alpha))
- \oint_C \frac{d\nu}{2\pi i} [\coth(2\nu) + \coth(2\nu + \eta) - \coth(\nu + \alpha)] \log(1 + a(\nu))
- \frac{1}{2} \log \frac{\det(1 - \hat{H}^+)}{\det(1 - \hat{H}^-)} + \frac{\coth(\alpha) \sinh(\eta)}{T},
\] (4.23)

where now \( h_z = \sinh(\eta) \coth(\alpha) \).

It is interesting to consider the case of fixed boundary conditions. For example,
fixing the boundary spin to \( \langle \sigma_z \rangle = -1 \) can be obtained from (4.23) by the \( h_z \to \infty, \alpha \to 0 \) limit. In this case \( \alpha \) is within the canonical contour and (4.23) has two diverging
terms. Using the NLIE (2.61) we get in this limit
\[
- \delta_{-\alpha} \log(1 + a(-\alpha)) + \frac{\coth(\alpha) \sinh(\eta)}{T} = - \frac{h_z}{T} + O(\alpha).
\] (4.24)

Substituting \( \alpha = 0 \) into the contour integral of (4.23) and using the representation
(2.66) for the bulk free energy density we get the relation
\[
\lim_{h_z \to \infty} \left( \frac{F_B}{T} + \frac{h_z}{T} \right) = F_B(\alpha = \eta, \beta = \infty) - f.
\] (4.25)

The right hand side describes the boundary free energy of a chain with one less sites
and longitudinal magnetic field \( h_z = \sinh(\eta) \coth(\eta) = \cosh(\eta) \). This is exactly what we
expect from the Hamiltonian (2.1) after we freeze one of the boundary spins and correct
for the diverging additive term.

An other interesting special case of (4.16) is when \( h_z = 0 \), but \( h_x \) is finite. This is
achieved by choosing \( \beta = 0 \) such that
\[
h_x = \frac{\sinh(\eta)}{\sinh(\alpha)}.
\] (4.26)

For this case we obtain
\[
\frac{F_B}{T} = \frac{1}{2} \frac{- \delta_{\Delta_{>1}}}{2} \log(2) - \delta_{-\alpha} \log(1 + a(-\alpha))
- \oint_C \frac{d\nu}{2\pi i} [\coth(2\nu) + \coth(2\nu + \eta) - \tanh(\nu) - \coth(\nu + \alpha)] \log(1 + a(\nu))
- \frac{1}{2} \log \frac{\det(1 - \hat{H}^+)}{\det(1 - \hat{H}^-)} + \frac{\coth(\alpha) \sinh(\eta)}{T}.
\] (4.27)

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The important case of the free boundary conditions \((h_x = h_z = 0)\) is obtained by substituting \(\alpha = i\pi/2\) into (4.23) or by taking the \(\alpha \to \infty\) limit of (4.27). In either case we get

\[
F_B/T = \frac{1 - \delta_{\Delta > 1}}{2} \log(2) - \frac{1}{2} \log \frac{\det(1 - \hat{H}^+)}{\det(1 - \hat{H}^-)}
- \oint_C \frac{d\nu}{2\pi i} \left[ \coth(2\nu) + \coth(2\nu + \eta) - \tanh(\nu) \right] \log(1 + a(\nu)).
\] (4.28)

4.3. Boundary magnetization

Here we compute the expectation values of the boundary spin operators using the relations

\[
\langle \sigma^a \rangle = \frac{\partial F_B}{\partial h^a}, \quad a = x, z.
\] (4.29)

Applying the chain rule we get

\[
\left( \langle \sigma_1^x \rangle \langle \sigma_1^z \rangle \right) = \left( \frac{\partial F_B}{\partial \alpha} \frac{\partial F_B}{\partial \alpha} \right) \left( \frac{\partial \alpha}{\partial \alpha} \frac{\partial \alpha}{\partial \alpha} \right).
\] (4.30)

The Jacobian is found to be

\[
\left( \frac{\partial \alpha}{\partial \alpha} \frac{\partial \alpha}{\partial \alpha} \right) = \frac{\sinh(\alpha) \cosh(\beta)}{\sinh(\eta) \sinh^2(\beta) + \cosh^2(\alpha)} \begin{pmatrix}
-\sinh(\beta) \sinh(\alpha) & -\cosh(\alpha) \sinh(\alpha) \\
\cosh(\alpha) \cosh(\beta) & -\sinh(\beta) \cosh(\beta)
\end{pmatrix},
\] (4.31)

and the \(\alpha, \beta\)-derivatives are

\[
\frac{\partial F_B}{\partial \alpha} = \frac{1}{\sinh^2(\alpha) \sinh(\eta)} + T \delta_{-\alpha} \frac{a'(-\alpha)}{1 + a(-\alpha)} - T \oint_C \frac{d\nu}{2\pi i} \log(1 + a(\nu))
\]

\[
\frac{\partial F_B}{\partial \beta} = \frac{1}{\cosh^2(\beta) \sinh(\eta)} + T \delta_{-\beta - i\pi/2} \frac{a'(-\beta - i\pi/2)}{1 + a(-\beta - i\pi/2)} + T \oint_C \frac{d\nu}{2\pi i} \log(1 + a(\nu)).
\] (4.32)

If needed, the derivatives of the auxiliary function can be computed using the NLIE (2.61).

5. High temperature limit

In this section we compute the high temperature limit of the boundary free energy. This provides a highly non-trivial check of the final results of the previous section.

First we compute the high \(T\) limit from the definition of the partition function. In any finite volume we have to first order in \(1/T\)

\[
Z = \text{Tr} e^{-H/T} = \text{Tr} 1 - \text{Tr} H/T + O(T^{-2}).
\] (5.1)
In the normalization (2.1) this gives
\[ Z = 2^L (1 + T^{-1} \Delta (L - 1)) + \mathcal{O}(T^{-2}), \quad F = -TL \log 2 - \Delta (L - 1) + \mathcal{O}(T^{-1}). \]  
(5.2)

The bulk piece is \( f = -T \log(2) - \Delta + \mathcal{O}(T^{-1}) \) and we can read off the boundary contribution
\[ \lim_{T \to \infty} 2F_B = \Delta. \]  
(5.3)

This constant is not physical, it merely represents the additive normalization of the bulk term in the Hamiltonian. Nevertheless we re-derive it from the general result (4.16).

For simplicity we consider the case when \( \alpha, \beta \) lie outside the contour, but the manipulations will be valid for arbitrary \( \Delta \). In the high temperature limit we have from (2.61) \( \lim_{T \to \infty} a(\lambda) = 1 \). The first correction is easily found from (2.61). Defining
\[ a(\lambda) = 1 + T^{-1} G(\lambda) + \mathcal{O}(T^{-2}) \]  
we get the linear integral equation
\[ G(\lambda) = -\frac{2 \sinh^2(\eta)}{\sinh(\lambda) \sinh(\lambda + \eta)} + \int_C \frac{d\nu}{2\pi i} \varphi(\lambda - \nu) \frac{G(\nu)}{2}. \]  
(5.5)

The solution is
\[ G(\lambda) = \sinh(\eta) \left[ \frac{\cosh(\lambda + \eta)}{\sinh(\lambda + \eta)} + \frac{\cosh(\lambda - \eta)}{\sinh(\lambda - \eta)} - 2 \frac{\cosh(\lambda)}{\sinh(\lambda)} \right]. \]  
(5.6)

This is obtained iteratively from (5.5) using contour integral manipulations. The solution (5.6) can be checked by substituting it back into (5.5) and noting that in the contour integral the only singularity is a simple pole at \( \nu = 0 \), whose contribution is \(-\sinh(\eta) \varphi(\lambda)\).

As a first step we prove that \( \lim_{T \to \infty} F_B/T = 0 \). To this order it is enough to substitute \( a \equiv 1 \) into (4.16). This gives immediately
\[ \lim_{T \to \infty} F_B/T = -\lim_{T \to \infty} \frac{1}{2} \log \det \left( 1 - \hat{H}^+ \right) \det \left( 1 - \hat{H}^- \right). \]  
(5.7)

The Fredholm determinants can be analyzed using the expansion (4.19). To lowest order in \( T^{-1} \) the weight function in the kernels (4.15) becomes \( a/(1 + a) = 1/2 \). Each trace is a multiple contour integral over functions that are free of poles within \( C \), thus in this limit both determinants evaluate to unity, and we get indeed \( \lim_{T \to \infty} F_B/T = 0 \).

To get the first corrections we use the approximations
\[ \log(1 + a(\lambda)) = \log(2) + \frac{1}{2T} G(\lambda) + \mathcal{O}(T^{-2}) \quad \frac{a(\lambda)}{1 + a(\lambda)} = \frac{1}{2} + \frac{1}{4T} G(\lambda) + \mathcal{O}(T^{-2}) \]  
(5.8)

In the expansion (4.19) only the term with \( n = 1 \) contributes, leading to
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\[
-\frac{1}{2} \log \frac{\det(1 - \hat{H}^+)}{\det(1 - \hat{H}^-)} = \frac{1}{2} \int_C \frac{d\lambda}{2\pi i} \frac{1}{4T} G(\lambda) \varphi(2\lambda) + O(T^{-2}) \\
= -\frac{1}{2T} \cosh(\eta) + O(T^{-2}).
\]

It follows that

\[
\lim_{T \to \infty} F_B = -\frac{1}{2} \cosh(\eta) + (\coth(\alpha) + \tanh(\beta)) \sinh(\eta) \\
- \oint_C \frac{d\nu}{2\pi i} \left[ \coth(2\nu) + \coth(2\nu + \eta) - \coth(\nu + \alpha) - \tanh(\nu + \beta) \right] \frac{G(\lambda)}{2} \\
= -\frac{1}{2} \cosh(\eta) + \cosh(\eta) = \frac{1}{2} \cosh(\eta).
\]

This is in accordance with (5.3).

Higher order corrections in $1/T$ could be obtained by taking further derivatives of the NLIE and thus by computing a number of simple contour integrals. The calculations would be analogous to the high-$T$ expansion of the free energy itself [32]. We do not pursue this direction here, because real space calculations for the high temperature expansion are considerably simpler. For the sake of completeness we give the second term:

\[
F_B = \Delta^2 + 1 \left[ \frac{2 + \Delta^2}{4} - \frac{h_x^2 + h_z^2}{2} \right] + O(T^{-2}).
\]

(5.10)

(5.11)

6. The $T \to 0$ limit

Here we investigate the low temperature behaviour of the boundary free energy.

In the $T \to 0$ limit $F_B$ becomes the boundary energy $E_B$ of the ground state, which is defined as

\[
2E_B = \lim_{L \to \infty} (E_0(L) - e_0L),
\]

where $E_0(L)$ is the finite volume ground state energy and $e_0$ is the ground state energy density. Once again we assumed identical boundary conditions at the two ends of the chain.

For $E_B$ a number of results have been already derived, both for purely longitudinal [12, 13] and arbitrary boundary fields [9, 23–25]. The final results depend on the root content of the ground state: depending on the parameters there can be boundary bound states, that are represented by special Bethe roots. Therefore, the discussion of the boundary energy has to be performed carefully, as it was done in the works cited above.

In this section we compute $E_B$ in both regimes and reproduce earlier results in the literature. In the massive regime we also investigate the first low-$T$ correction terms: we argue that in most cases there is linear term in $T$ whose coefficient is exactly obtained. In the massless case we discuss the earlier predictions of QFT methods.
6.1. The massive regime

It is useful to introduce the $b$-$\bar{b}$ formulation [31, 54] of the NLIE. First we make use of the coordinate transformation $\lambda = ix$. We define $\bar{a}(x) = a(ix)$. The integral equation becomes

$$\log \bar{a}(u) = 2\beta \frac{\sinh \eta}{\sin(u) \sin(u - i\eta)} - \int_C \frac{d\nu}{2\pi \sin(u - \nu + i\eta) \sin(u - \nu - i\eta)} \log(1 + \bar{a}(\nu)). \quad (6.1)$$

We define the functions

$$b(x) = \lim_{\varepsilon \to 0} \bar{a}(x - i\eta/2 + i\varepsilon) \quad \bar{b}(x) = \lim_{\varepsilon \to 0} \bar{a}^{-1}(x + i\eta/2 - i\varepsilon) \quad (6.2)$$

and

$$\mathcal{B}(x) = 1 + b(x) \quad \mathcal{B}(x) = 1 + \bar{b}(x). \quad (6.3)$$

These functions satisfy the symmetry properties

$$b(x) = b(-x) = b^*(x) \quad \mathcal{B}(x) = \mathcal{B}(-x) = \mathcal{B}^*(x). \quad (6.4)$$

The NLIE can be transformed to the form (for a detailed derivation see [64])

$$\log b(x) = -\frac{2 \sinh(\eta)}{T} s(x) + \int \frac{dy}{2\pi} \kappa(x - y) \log \mathcal{B}(y) \quad \text{for} \quad |\Im(x)| < \eta$$

$$- \lim_{\varepsilon \to 0} \int \frac{dy}{2\pi} \kappa(x - y - 2i(\eta - \varepsilon)) \log \mathcal{B}(y), \quad (6.5)$$

where

$$s(x) = 1 + 2 \sum_{n=1}^\infty \frac{\cos(2n\pi x)}{\cosh(\eta n)}, \quad (6.6)$$

and

$$\kappa(x) = \sum_{k=-\infty}^{\infty} \frac{e^{-|k|\eta}}{\cosh(k\eta)} e^{2ikx}. \quad (6.7)$$

Note that $\kappa$ is well defined only if $|\Im(x)| < \eta$ and it has a pole at $x = \pm i\eta$. This is the reason why this set of auxiliary functions and the NLIE are only defined through the $\varepsilon \to 0$ limit.

It follows from the NLIE that in the $T \to 0$ limit $\bar{a}(x)$ becomes exponentially large/small if $x$ is in the upper/lower half-plain. For $x \in \mathbb{R}$ we have $|\bar{a}(x)| = 1$ for arbitrary temperatures (this follows from the original definition (2.48) and the symmetry of the Bethe roots), nevertheless the function $\bar{a}(x)$ does not have a finite $T \to 0$ limit. An exception is given by the special point $x = \pi/2$ for which we have $\bar{a}(\pi/2) = a(i\pi/2) = 1$ at arbitrary temperatures.

For the limiting behaviour of the $b$-$\bar{b}$ functions we have

$$\lim_{T \to 0} \left(T \log(b(x))\right) = \lim_{T \to 0} \left(T \log(\bar{b}(x))\right) = -2 \sinh(\eta) s(x). \quad (6.8)$$

Therefore the original contour integrals over any function $f(u)$ have the limiting behaviour

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\[
\lim_{T \to 0} \left[ T \int_C \frac{du}{2\pi i} f(u) \log(1 + a(u)) \right] = 2 \sinh(\eta) \lim_{\varepsilon \to 0} \left[ \int \frac{dx}{2\pi} s(x - i\varepsilon) f(i\varepsilon - \eta + 2 + \varepsilon) \right]. \quad (6.9)
\]

We are now in the position to compute the \( T \to 0 \) limit of the formula (4.16). It can be seen that the Fredholm determinants remain bounded, because their weight functions converge to finite values (the limiting value of the ratio will be computed at the end of this subsection). Therefore the \( T \to 0 \) limit of the free energy is determined by the constants and the simple integrals.

First we consider the case when there are no boundary bound states, that is, when \( \alpha \) and \( \beta \) lie outside the physical strip. Using (6.9) we get

\[
\lim_{T \to 0} F_B = \sinh(\eta) \left[ \coth(\alpha) + \tanh(\beta) + 2 \lim_{\varepsilon \to 0} \int \frac{dx}{2\pi} s(x - i\varepsilon) \left[ \coth(2ix - \eta + 2\varepsilon) \right. \right.
\]

\[
+ \coth(2ix + 2\varepsilon) - \coth(ix - \eta/2 + \alpha + \varepsilon) - \tanh(ix - \eta/2 + \beta + \varepsilon) \right]\]. \quad (6.10)

The integrals can be evaluated using the following identities, that hold for an arbitrary \( \gamma \in \mathbb{R} \):

\[
\int_{-\pi/2}^{\pi/2} \frac{dx}{2\pi} s(x) \coth(ix + \gamma) = \text{sign}(\gamma) \sum_{n=-\infty}^{\infty} \frac{e^{-2|n\gamma|}}{2 \cosh(n\eta)}
\]

\[
\int_{-\pi/2}^{\pi/2} \frac{dx}{2\pi} s(x) \coth(2ix + \gamma) = \text{sign}(\gamma) \sum_{n=-\infty}^{\infty} (1 + (-1)^n) e^{-|n\gamma|} \left( 1 + \frac{1}{4 \cosh(n\eta)} \right)
\]

\[
\int_{-\pi/2}^{\pi/2} \frac{dx}{2\pi} s(x) \tanh(ix + \gamma) = \text{sign}(\gamma) \sum_{n=-\infty}^{\infty} (-1)^n e^{-2|n\gamma|} \frac{1}{2 \cosh(n\eta)}.
\]

Putting everything together we obtain the following formula for the boundary energy:

\[
E_B = \lim_{T \to 0} F_B = \sinh(\eta)(\epsilon_0 + \epsilon_\alpha + \epsilon_\beta), \quad (6.12)
\]

with

\[
\epsilon_0 = \frac{1}{2} \sum_{n=-\infty}^{\infty} \frac{(1 - e^{-|n\eta|})(1 + (-1)^n)}{\cosh(n\eta)} = 2 \sum_{n=1}^{\infty} \frac{1 - e^{-2n\eta}}{\cosh(2n\eta)} \quad (6.13)
\]

and

\[
\epsilon_\alpha = \coth(\alpha) - \text{sign}(\alpha - \eta/2) \left[ 1 + 2 \sum_{n=1}^{\infty} \frac{e^{-|2\alpha-\eta|n}}{\cosh(n\eta)} \right]
\]

\[
\epsilon_\beta = \tanh(\beta) - \text{sign}(\beta - \eta/2) \left[ 1 + 2 \sum_{n=1}^{\infty} (-1)^n e^{-|2\beta-\eta|n} \frac{1}{\cosh(n\eta)} \right]. \quad (6.14)
\]

Expression (6.12) agrees with the earlier result for this case published in [9]: it coincides with formula (5.4.47) after correcting for the differences in the definition of the Hamiltonian, including certain signs of the boundary parameters.

The case with boundary bound states can be treated similarly. For example consider the case when \( \alpha \) is within the physical strip, and we need to evaluate the extra term \( T \log(1 + a(-\alpha)) = T \log(1 + \tilde{a}(-i\alpha)) \). It can be seen from (6.5) that if \( \alpha < 0 \) then

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this term becomes exponentially small, but it gives a finite contribution when $\alpha > 0$. In the latter case the NLIE yields

$$\lim_{T \to 0} \left[ T \log(1 + a(-\alpha)) \right] = \lim_{T \to 0} \left[ T \log a(-\alpha) \right] = -\lim_{T \to 0} \left[ T \log b(i(\alpha - \eta/2)) \right]$$

$$= 2 \sinh(\eta) s(i(\alpha - \eta/2)) = 2 \sinh(\eta) \left( 1 + 2 \sum_{n=1}^{\infty} \frac{\cosh(n\eta - 2n\alpha)}{\cosh(\eta)} \right). \quad (6.15)$$

This term needs to be added to expression (6.12) if $0 < \alpha < \eta/2$. A similar contribution has to be added when $0 < \beta < \eta/2$.

An important test of the results is that the boundary energy should be invariant with respect to the spin flips $h_z \rightarrow -h_z$ and/or $h_x \rightarrow -h_x$, which corresponds to $\alpha, \beta \rightarrow -\alpha, -\beta$. A simple calculation shows that if $\alpha$ and $\beta$ lie outside the physical strip, then the functions $e_1(\alpha)$ and $e_2(\beta)$ are indeed symmetric. On the other hand, if for example $|\alpha| < \eta/2$ then $E_B$ becomes symmetric after we add the extra contribution (6.15) when $\alpha > 0$. The total boundary energy is thus always symmetric.

In view of these symmetry considerations the boundary energy is always described by formula (6.12) with $e_0$ given by (6.13) but $e_{\alpha, \beta}$ replaced by

$$e_\alpha = -\coth(|\alpha|) + 1 + 2 \sum_{n=1}^{\infty} \frac{e^{-(2|\alpha|+\eta)n}}{\cosh(n\eta)}$$

$$e_\beta = -\tanh(|\beta|) + 1 + 2 \sum_{n=1}^{\infty} \frac{(-1)^n e^{-(2|\beta|+\eta)n}}{\cosh(n\eta)}. \quad (6.16)$$

The specific case of free boundary conditions is obtained by evaluating the low-$T$ limit of the integrals in (4.28), or simply taking the $\alpha \rightarrow \infty$, $\beta \rightarrow 0$ limit of (6.12). Either way we get

$$E_B = \sinh \eta \left[ 1 + 2 \sum_{n=1}^{\infty} \frac{(1 - e^{-2n\eta})}{\cosh(2n\eta)} + 2 \sum_{n=1}^{\infty} \frac{(-1)^n e^{-n\eta}}{\cosh(n\eta)} \right]. \quad (6.17)$$

After correcting for the differences in the definition of the Hamiltonian this coincides with the formula (32) presented in [13].

It is also possible to compute the first low-$T$ correction to $E_B$. Again, we first consider the case when $\alpha, \beta$ lie outside the physical strip. The NLIE (6.5) implies that for very low temperatures the correction terms to the simple integrals will be exponentially small. Thus the leading correction is a linear term given by

$$F_B = E_B + T \left( \log(2) - \frac{1}{2} \lim_{T \to 0} \log \frac{\det (1 - \hat{H}^+)}{\det (1 - \hat{H}^-)} \right) + \ldots. \quad (6.18)$$

The limit of the Fredholm determinants is computed as follows. The weight function $\tilde{a}(\nu)/(1 + \tilde{a}(\nu))$ becomes exponentially small on the upper contour, therefore it is enough to consider the integrations over the lower contour on which $\tilde{a}(\nu)/(1 + \tilde{a}(\nu)) \rightarrow 1$. We get
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\[
\frac{\det (1 - \hat{H}^+)}{\det (1 - \hat{H}^-)} \to \frac{\det (1 - \hat{H}_0^+)}{\det (1 - \hat{H}_0^-)},
\]

where \(H_0^\pm\) are integral operators that act on functions defined on the segment \([-\pi/2...\pi/2] - ia, \ a < \eta/2\) as

\[
(\hat{H}_0^\pm (g))(x) = -\int_{-\pi/2}^{\pi/2} \frac{du}{2\pi} \frac{\varphi(x-u) \pm \varphi(x+u-2ia)}{2} g(u)
\]

\[
= -\int_{-\pi/2}^{\pi/2} \frac{du}{2\pi} \varphi(x-u) g(u) \pm g(-u-2ia) / 2.
\]

The overall minus sign in front of the integrals originates in the transition from the contour integrals to the real integrals.

The determinants can be evaluated in Fourier space. The integral operator couples the Fourier modes \(g_n\) and \(g_{-n}\) for any \(n > 1\), the matrices \(1 - \hat{H}_0^\pm\) are thus block-diagonal with \(2 \times 2\) blocks, except for the zero Fourier mode. The sign difference between the two operators affects the two off-diagonal matrix elements in the \(2 \times 2\) blocks, therefore all sub-determinants are actually equal. The difference between the two determinants is thus only in the zero mode, and we get

\[
\frac{\det (1 - \hat{H}_0^+)}{\det (1 - \hat{H}_0^-)} = \frac{1 + \int_{-\pi/2}^{\pi/2} \frac{du}{2\pi} \varphi(x-u) + \varphi(x+u-2ia)}{1 + \int_{-\pi/2}^{\pi/2} \frac{du}{2\pi} \varphi(x-u) - \varphi(x+u-2ia)} = 1 + \int_{-\pi/2}^{\pi/2} \frac{du}{2\pi} \varphi(u) = 2.
\]

The leading term to the boundary free energy is thus

\[
F_B = E_B + T \log(2) + \ldots.
\]

In those cases when \(\alpha\) or \(\beta\) lie within the physical strip we need to consider the low-\(T\) corrections to the extra terms \(\log(1 + a(\alpha))\) and \(\log(1 + a(\beta - i\pi/2))\). However, the NLIE implies that the corrections will be exponentially small, except the special case of \(\log(1 + a(-i\pi/2)) = \log(2)\) which holds for arbitrary temperatures. This is encountered only when \(h_z = 0\) and according to (4.27) it results in

\[
F_B = E_B - T \frac{\log(2)}{2} + \ldots.
\]

In the massive regime the \(O(T)\) terms can be summarized as

\[
F_B = E_B + T \log(2) \left( \frac{1}{2} - \delta_{h_z=0} \right) + \ldots,
\]

where the dots denote corrections that are exponentially suppressed in \(1/T\).

### 6.2. The massless regime

Now \(\eta = i\gamma\) with \(\gamma \in \mathbb{R}\). We will also use \(\alpha = i\tilde{\alpha}\) such that \(\tilde{\alpha} \in \mathbb{R}\).

The \(b - \bar{b}\) formulation of the NLIE is introduced as follows. We define

\[
\text{https://doi.org/10.1088/1742-5468/aae5a5}
\]

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\[ \mathbf{b}(x) = \lim_{\varepsilon \to 0} a(x + i\gamma/2 + i\varepsilon) \quad \mathbf{b}(x) = \lim_{\varepsilon \to 0} a^{-1}(x - i\gamma/2 - i\varepsilon), \]  
(6.25)

and \( \mathcal{B} - \bar{\mathcal{B}} \) are given by (6.3). The NLIE can be transformed into the form [31, 64]

\[ \log \mathbf{b}(x) = -\frac{2\sin(\gamma)}{T} d(x) + \int \frac{dy}{2\pi} \kappa(x - y) \log \mathcal{B}(y) \]
\[ - \lim_{\varepsilon \to 0} \int \frac{dy}{2\pi} \kappa(x - y - 2i(\eta - \varepsilon)) \log \bar{\mathcal{B}}(y), \]
(6.26)

where now

\[ d(x) = \frac{\pi}{\gamma \cosh(\pi x/\gamma)} \]  
(6.27)

and

\[ \kappa(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{\sinh((\pi/2 - \gamma)k)}{2 \cosh(\gamma k/2) \sinh((\pi/2 - \gamma/2)k)} e^{ikx}. \]
(6.28)

The asymptotic behaviour of the auxiliary functions is similar to that of the massive case, nevertheless there are important differences that result in other types of correction terms. The NLIE implies that in the low-\( T \) limit \( a(x) \) becomes exponentially large/small for \( x \) in the lower/upper half-planes, respectively. However, for any fixed \( T \) the asymptotics is always given by

\[ \lim_{g(x) \to \pm\infty} a(x) = 1. \]
(6.29)

For any finite \( T \) there is a crossover regime in \( x \) where the source term of the NLIE (6.26) is \( O(1) \), this happens when

\[ |x| \approx x_0 = \frac{\gamma}{\pi} \log \left[ \frac{4\pi \sin(\gamma)}{T \gamma} \right]. \]
(6.30)

In this regime a \( T \)-independent asymptotic NLIE can be written down for a shifted rapidity variable \( x - x_0 \), whose solution describes a kink that moves with \( T \) in rapidity space [32]. The logarithmic dependence implies that depending the problem at hand the temperature must be chosen extremely low to reach the asymptotic regime. This will have a relevance to our numerical data for \( F_B \).

Now we compute the boundary energy in this regime. Once again the \( T \to 0 \) limit of \( F_B \) will be given by the simple integrals and the constant terms, because the Fredholm determinants will remain regular and thus they only contribute an \( o(1) \) term to \( F_B \). The boundary parameter \( \beta \) is real and thus in this regime the special point \( -\beta - i\pi/2 \) is always outside the canonical contour. Therefore

\[ E_B = \lim_{T \to 0} F_B = - \lim_{T \to 0} \delta_{\alpha} \log(1 + a(-\alpha)) + i(\coth(\alpha) + \tanh(\beta)) \sin(\gamma) \]
\[ - \lim_{T \to 0} \int_\gamma^{2\gamma} \frac{d\nu}{2\pi} \left[ \coth(2\nu) + \coth(2\nu + \eta) - \coth(\nu + \alpha) - \tanh(\nu + \beta) \right] \log(1 + a(\nu)). \]
(6.31)

In the following we concentrate on the case when \( \alpha \) is outside the physical strip. It follows from the NLIE that in the \( T \to 0 \) limit the leading contribution comes from the lower contour and it reads

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\[ E_B = + i(\coth(\alpha) + \tanh(\beta)) \sin(\gamma) - \lim_{\epsilon \to 0} \int_{-\infty}^{\infty} \frac{d\nu}{2\pi i} \left[ \coth(2\nu - i\gamma) \right. \]
\[ + \coth(2\nu + 2i\epsilon) - \coth(\nu + \alpha - i\gamma/2) - \tanh(\nu + \beta - i\gamma/2) \left. \right] 2\sin(\gamma) d(x). \]  
\hspace{16.5cm} (6.32) 

After symmetrizing the integral and using
\[ \lim_{\epsilon \to 0} \left( \coth(2\nu + 2i\epsilon) - \coth(2\nu - 2i\epsilon) \right) = -\pi \delta(\nu) \]  
\hspace{16.5cm} (6.33) 
we get
\[ E_B = \sin(\gamma) \left\{ i(\coth(\alpha) + \tanh(\beta)) + \frac{d(0)}{2} - \int_{-\infty}^{\infty} \frac{dx}{2\pi i} \left[ \frac{\sin(2\nu)}{\sinh(2\nu - i\gamma)\sinh(2x + i\gamma)} \right. \right. \]
\[ - \frac{\sin(2\alpha - i\gamma)}{\sinh(x + \alpha - i\gamma/2)\sinh(x - \alpha + i\gamma/2)} - \frac{\sin(2\beta - i\gamma)}{\cosh(x + \beta - i\gamma/2)\cosh(x - \beta + i\gamma/2)} \left. \right] d(x) \right\}. \]  
\hspace{16.5cm} (6.34) 

The case of free boundary conditions is obtained by setting \( \alpha = i\pi/2 \) and performing the limit \( \beta \to \infty \). In this case we obtain
\[ E_B = \sin(\gamma) \frac{d(0)}{2} - \sin(\gamma) \int_{-\infty}^{\infty} \frac{dx}{2\pi} \left[ \frac{\sin(2\nu)}{\sinh(2\nu - i\gamma)\sinh(2x + i\gamma)} \right. \]
\[ - \frac{\sin(\gamma)}{\cosh(x - i\gamma/2)\cosh(x + i\gamma/2)} \left. \right] d(x). \]  
\hspace{16.5cm} (6.35) 

It is an important task to consider the first low-\( T \) corrections in \( F_B \) and to compare to predictions from QFT. The works \([45, 47, 65]\) treated the case of free boundary conditions using conformal field theory (CFT) and bosonization techniques. These papers concentrated on the boundary contribution to the total susceptibility, therefore they computed \( F_B \) in the general case with a finite \( h \) bulk magnetic field. Their formulas should describe the low-\( T \) behaviour of our results for \( h = 0 \). Correcting for the differences in the definitions of the Hamiltonian and \( F_B \) their result reads
\[ F_B = E_B + \frac{\lambda \Gamma(K)\Gamma(1 - 2K)}{2\Gamma(1 - K)} \left( \frac{2\pi T}{v} \right)^{2K-1} + \mathcal{O}(T^2), \]  
\hspace{16.5cm} (6.36) 
where
\[ K = \frac{1}{1 - \gamma/\pi} \]
\[ v = \frac{2K \sin(\pi/K)}{K - 1} \]
\[ \lambda = \frac{4K \Gamma(K) \sin(\pi/K)}{\pi \Gamma(2 - K)} \left( \frac{\Gamma(1 + \frac{1}{2K-2})}{2\sqrt{\pi} \Gamma(1 + \frac{K}{2K-2})} \right)^{2K-2}. \]  
\hspace{16.5cm} (6.37) 

Most importantly they found that there is no linear term in \( F_B \).

At present we are not able to confirm or disprove the above prediction. The behaviour of the integrals and Fredholm-determinants is considerably more involved in the massless regime than in the massive. On the one hand, if we choose \( \mathcal{C} \) to be a compact contour then \( \mathcal{C} \) needs to be changed as we lower the temperature. On the other hand,
if we choose \( \mathcal{C} \) to be the union of two straight lines, then both the single integrals and the Fredholm determinants become ill behaving. We plan to return to this problem in future research.

7. The XXX limit

Here we compute the boundary free energy at the isotropic point. In principle we could repeat the whole calculation using the \( R \) and \( K \) matrices of the XXX model, but it is easier to take the limits of the final formulas. The boundary free energy is a continuous function of \( \Delta \), and we choose to approach \( \Delta = 1 \) from the massless regime.

It is known that with the parametrization \( \Delta = \cos(\gamma) \) the \( \gamma \to 0 \) limit leads to a re-scaling of the rapidity variables according to
\[
\lambda_{\text{XXX}} \rightarrow \gamma \lambda_{\text{XXX}},
\]
(7.1)
such that the \( \lambda_{\text{XXX}} \) become the finite variables of the XXX model.

After this re-scaling the NLIE (2.61) takes the form
\[
\log a(\lambda) = \frac{1}{T} \frac{2}{\lambda(\lambda + i)} + \int_{\mathcal{C}} \frac{d\nu}{2\pi i} \tilde{\varphi}(\lambda - \nu) \log(1 + a(\nu)),
\]
(7.2)
where
\[
\tilde{\varphi}(u) = -\frac{2}{u^2 + 1}
\]
(7.3)
and the contour \( \mathcal{C} \) encircles the real line such that it remains in the physical strip \( |\Im(\lambda)| < 1/2 \). In practice \( \mathcal{C} \) can be chosen as the union of \( \mathbb{R} - i\kappa \) and \( \mathbb{R} + i\kappa \) with \( \kappa < 1/2 \).

The re-scaling of the boundary parameters can be read off (2.23). Finite fields are obtained with the re-scaling \( \alpha \to i\gamma\hat{\alpha} \) and keeping \( \beta \) finite, such that in the XXX limit
\[
h_x = \frac{1}{\hat{\alpha} \cosh(\beta)} \quad h_z = \frac{1}{\hat{\alpha} \tanh(\beta)},
\]
(7.4)
where \( \hat{\alpha}, \beta \in \mathbb{R} \). It can be seen that the amplitude of the magnetic field is \( 1/|\hat{\alpha}| \) and the \( \beta \) parameter only describes an angle in the \( z - x \) plain.

Performing the scaling on (4.16) we obtain the boundary free energy as
\[
F_B/T = \frac{1}{2} \log(2) - \oint_{\mathcal{C}} \frac{d\nu}{2\pi i} \left[ \frac{1}{2\nu} + \frac{1}{2\nu + i} - \frac{1}{\nu + i\hat{\alpha}} \right] \log(1 + a(\nu))
\]
\[
- \delta_{-i\hat{\alpha}} \log(1 + a(-i\hat{\alpha})) - \frac{1}{2} \log \frac{\det \left( 1 - \hat{H}^+_{\text{XXX}} \right)}{\det \left( 1 - \hat{H}^-_{\text{XXX}} \right)} + \frac{1}{aT},
\]
(7.5)
where \( \hat{H}^\pm_{\text{XXX}} \) are integral operators that act as
\[
\left( \hat{H}^\pm_{\text{XXX}}(g) \right)(x) = \int_{\mathcal{C}} \frac{du}{2\pi} \frac{a(u)}{1 + a(u)} \tilde{\varphi}(x - u) \pm \tilde{\varphi}(x + u) g(u).
\]
(7.6)
The ratio of Fredholm determinants is given alternatively by (4.19) with the replacements
\[
\int \frac{d\lambda_j}{2\pi i} \tilde{\phi}(\ldots) \quad \rightarrow \quad \int \frac{d\lambda_j}{2\pi} \tilde{\phi}(\ldots).
\] (7.7)

It is an important consistency check of the scaling procedure that the \(\beta\)-dependent contributions vanished, signaling the \(SU(2)\)-invariance of the problem.

Free boundary conditions are obtained in the \(\tilde{\alpha} \rightarrow \infty\) limit, when all \(\tilde{\alpha}\)-dependent terms disappear from (7.5).

8. The ferromagnetic chain

The parameter choice \(\Delta < -1\) describes the ferromagnetic spin chain, and here we explain how the previous formulas can be used for \(\Delta < 0\) as well.

Let us consider the total free energy in any finite volume of even length, and let us denote it by \(F(\Delta, T)\). Performing a similarity transformation with the operator \(U = \prod_{j=1}^{L/2} \sigma_{2j-1}^z\) we get the relation [30]:
\[
F(\Delta, T) = F(-\Delta, -T).
\] (8.1)

Negative values of \(\Delta\) can thus be treated by using negative values of \(T\) in our formalism. The main equations (2.61) and (4.16) are analytic in the parameter \(1/T\), therefore they can be continued naturally to the negative regime. This was already demonstrated in [66].

Naturally, the low-\(T\) behaviour of \(F_B\) is quite different in the ferromagnetic regime. In the case of free boundary conditions the two ground states are the ferromagnetic
reference states, such that \( E_B = \lim_{T \to 0} F_B = 0 \). In the case of finite boundary fields there can be boundary bound states, that give a finite contribution to \( E_B \).

These results can be obtained from our formulas; the low-\( T \) behaviour of the NLIE (2.61) can be studied similarly to the anti-ferromagnetic case. A \( b-b \) formulation can be written down similar to (6.5), but the source terms and integration kernels will be different. We omit the details of these calculations, because the main focus of this work is the anti-ferromagnetic chain.

9. Numerical investigations

In this section we numerically evaluate the exact formulas for \( F_B \). We only set a modest goal of giving a few examples of the numerical data; the complete exploration of the behaviour of \( F_B \) as a function of the temperature, the anisotropy, and the two boundary fields requires a separate study.

The NLIE (2.61) can be implemented easily in both the massive and massless regimes. An important point is the choice of the contour \( \mathcal{C} \). For \( \Delta > 1 \) we chose it to be the union of the segments \([-i\pi/2 + a \ldots i\pi/2 + a] \) and \([-i\pi/2 - a \ldots i\pi/2 - a] \) with \( a < \eta/2 \). In the massless regime the NLIE can be solved on the usual contour which is the union of \( \mathbb{R} + ia \) and \( \mathbb{R} - ia \) with \( a < \cos^{-1}(\Delta)/2 \). In our implementation we used the original \( a \)-formulation and the NLIE could be solved with iteration up to low temperatures of order \( T = 10^{-2} \). An important point is that the function \( \log(1 + a(\lambda)) \) has to be continuous in \( \lambda \), and artificial jumps of \( 2\pi i \) produced by the numerics have to be corrected.

Having found the numerical solution for \( a(\lambda) \) the integrals and the Fredholm determinants in (4.16) can be evaluated too. The determinants can be calculated by discretizing the integral operators and taking the determinant of the resulting matrix; this can be worked out even for curved contours. This is in fact required in the massless regime, where the expressions in (4.16) have weak convergence properties if \( \mathcal{C} \) is the union of the two straight lines as explained above. Instead, we considered an elliptic curve centered at \( \lambda = 0 \), where the major axis is large enough to include all Bethe roots of the QTM, and the minor axis is small enough so that the ellipse fits into the physical strip. This way the numerical data became convergent and stable with respect to changing the parameters of the ellipse.

As a first test of our results we compared them to exact diagonalization. We computed the partition function (2.2) on a finite chain and computed the boundary contribution as

\[
2F_B(L) = F_{ED}(L) - fL,
\]

where \( f \) is the exact value of the free energy density calculated from the NLIE (2.61). We performed this procedure on finite chains up to \( L = 12 \) and \( L = 13 \), and for various values of the parameters \( T \) and magnetic fields. It was observed that \( F_B(L) \) converged well for high or intermediate temperatures, when the correlation length in the system is relatively small. On the other hand, convergence was worse for lower temperatures, especially in the massless regime, as it was expected. We also observed that the
convergence depends strongly on the values of the magnetic fields. Examples for the numerical data are shown in tables 2 and 3.

Whereas exact diagonalization confirmed our data for intermediate and large temperatures, there were always sizable differences for small temperatures due to the large finite size effects. In order to test our formulas at low-$T$ we also compared them to unpublished numerical results obtained using DMRG, in the case of free boundary conditions. This data was produced and sent to us by Sirker, for which we are very grateful. The DMRG data confirmed the correctness of our formulas down to temperatures of order $T \approx 10^{-2}$.

In order to explore the temperature dependence of $F_B$ we produced numerical data for specific values of the anisotropy and the boundary magnetic fields. We found that as a function of $T$ there can be a variety of behaviors.

In the case of free boundary conditions three examples are shown in figure 3. Here we plot $\tilde{F}_B \equiv F_B - \Delta/2$ for three different values of $\Delta$. The shift of $-\Delta/2$ was added so that all curves approach 0 in the high temperature limit; $\tilde{F}_B$ corresponds to the boundary free energy of the Hamiltonian without the additive term in the bulk piece. We found that for large anisotropy $\tilde{F}_B$ is a monotonically decreasing function, but for smaller $\Delta$ it develops a local minimum and a local maximum, see for example the curve with $\Delta = 1.4$ in figure 3. For $\Delta > 1$ the function $\tilde{F}_B$ always starts with a negative slope (corresponding to (6.24)). We observed that as we lower $\Delta$ the position of the local maximum stays approximately constant, but the local minimum is shifted towards smaller temperatures. We also plotted the curve for $\Delta = 0.7$ and found that it is increasing for small temperatures and has only a local maximum. We attempted to compare the data at $\Delta = 0.7$ to the QFT predictions, but we found a mismatch. Our

| $\Delta$ | $T$ | $F_B$ | $F_B L = 12$ | $F_B L = 13$ |
|---------|-----|-------|--------------|--------------|
| 0.5     | 0.1 | 1.20833 | 1.15943      | 1.27526      |
| 0.5     | 0.5 | 1.22386 | 1.22233      | 1.2248       |
| 0.5     | 1   | 1.17986 | 1.17986      | 1.17986      |
| 0.5     | 2   | 1.00888 | 1.00888      | 1.00888      |
| 2       | 0.1 | 3.52883 | 3.39913      | 3.55386      |
| 2       | 1   | 3.25907 | 3.25874      | 3.25923      |
| 2       | 2   | 3.08094 | 3.08094      | 3.08094      |
| −2      | 0.5 | 0.17376 | 0.17376      | 0.17376      |
| −2      | 1   | 0.34185 | 0.34185      | 0.34185      |
| −2      | 2   | 0.54549 | 0.54549      | 0.54549      |

| $\Delta$ | $T$ | $F_B$ | $F_B L = 12$ | $F_B L = 13$ |
|---------|-----|-------|--------------|--------------|
| 2       | 1   | 0.46150 | 0.59893      | 0.36490      |
| 2       | 2   | 0.64993 | 0.66270      | 0.64094      |
| 2       | 5   | 0.83512 | 0.83513      | 0.83512      |
current numerical programs could only reach the temperature regime of \( T \approx 10^{-2} \) and for this magnitude of \( T \) we still observed a linear growth in \( \tilde{F}_B \). It is possible that for much smaller temperatures the QFT result (6.36) becomes correct, and further numerical and/or analytical investigations are needed to check or disprove this.

We also evaluated \( \tilde{F}_B \) in the cases with finite boundary fields. Examples of the data can be seen in figure 4, where we plot \( \tilde{F}_B = F_B - \Delta/2 \) such that all curves tend to 0 in the high temperature limit. The horizontal dashed lines show the \( T \to 0 \) limit as calculated from (6.12)–(6.16).

10. Conclusions and discussion

In this paper we treated the open XXZ spin chain and derived exact results for the boundary free energy and boundary magnetization, with the final formulas being (4.16) and (4.30). Special cases of the general result were presented in section 4.2. In this section we discuss our results and the open problems.

One of the key elements of our computation is the conjectured overlap formula (3.4). In the diagonal case (longitudinal boundary fields) it can be proven by known methods, but for generic \( K \)-matrices we could only check it numerically at finite Trotter...
number. Its validity is also corroborated by the fact that the final results for $F_B$ agree with exact diagonalization and DMRG and they produce the correct high and low temperature limits. Nevertheless, an actual proof at finite Trotter number is desirable.

The overlap formula assumes that the Bethe roots of the eigenstates of the QTM display the pair structure. It was shown in [52] that the pair structure for the non-vanishing overlaps follows from the boundary Yang–Baxter relations. The proof of [52] was given for the case of the physical spin chain, but it can be extended readily to the inhomogeneous case of the QTM. However, there is a limitation: the bulk magnetic field $h$ of the physical chain has to be zero. A finite bulk field would lead to twisted boundary conditions for the QTM [31, 54] which would break the pair structure of the Bethe roots. The bulk magnetic field is only compatible with the diagonal $K$-matrices, which preserve the $U(1)$ symmetry of the model. Therefore, exact results for the overlaps with $h \neq 0$ can only exist in the diagonal case. Numerical calculations show that for $h \neq 0$ more Bethe states have non-zero overlaps, and not only those that are the continuous deformations of the Bethe states with the pair structure. Therefore we conclude that for $h \neq 0$ the structure of the overlaps is drastically different, and we can not expect a simple modification of (3.4). We remind that the exact overlaps $h \neq 0$ were actually derived already in [49], but the final results for $F_B$ were more cumbersome than our present formulas. In fact, the goal of deriving the Gaudin-like determinants was the primary motivation for this work.

In section 2.2 we explained that $F_B$ could be derived alternatively in the framework of TBA, but the resulting expressions would be considerably more complicated. For example, the Fredholm operators would act also on the string indices. Nevertheless it is desirable to pursue this approach as well. For the periodic system the equivalence of the QTM and the TBA is understood [33], and it is desirable to establish the relation also in the boundary problem. An advantage of the TBA approach is that it could provide $F_B$ also in the case of a finite bulk magnetic field, because it only uses statistical arguments [40, 41] and the magnetic field is only a parameter of the source term of the TBA. Combined with our present formulas this could lead to manageable expressions even at finite $h$.

It is an important task to compute the low-temperature behaviour of $F_B$ in the massless regime, which could confirm the field theoretical predictions. In section 6.2 we computed the boundary energy, but the computation of the first non-trivial correction is more involved. For the temperatures accessible to our present numerical programs ($T \approx 10^{-2} - 10^{-3}$) the boundary free energy seemed to have a linear growth, which contradicts the predictions. If the QFT result is still correct, it only describes $F_B$ on a much smaller temperature scale than expected. From an analytical point of view the treatment of the isotropic point would be especially interesting, because in this case $F_B$ is known to have logarithmic terms in $T$ [47]. The asymptotic analysis of the XXX case could be performed starting with formula (7.5).

In section 9 we demonstrated the numerical evaluation of the exact results. We have found a wide variety of behaviour as a function of the anisotropy, the boundary fields, and the temperature. Perhaps surprisingly it was found that $F_B$ can be a non-monotonic function of the temperature, and the sign of its derivative depends on all parameters. This is already reflected by the high temperature expansion (5.11), which shows that the $O(1/T)$ terms can be positive or negative as well. So far we only concentrated on
the numerics for $F_B$, but it would be desirable to compute the boundary magnetization, and the boundary contributions to the entropy and the specific heat as well. These quantities are given by different derivatives of $F_B$. The exploration of these quantities is left to further research.

Finally we comment on the extension of these results to other models. In those cases when there is a QTM formulation of the thermodynamics and the boundary $K$-matrices are also known, our methods could be applied; a crucial step would be to find the generalization of the overlap formula (3.4) using the techniques of [52]. An example could be the spin-1 XXZ chain, where both the QTM [67] and the Boundary-ABA [68, 69] are already worked out. We should note that there have been recent works dealing with impurity thermodynamics within the QTM framework [70, 71]. Possible relations to our results need to be explored by future works.

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