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Factorization of the finite temperature correlation functions of the XXZ chain in a magnetic field

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Abstract

We present a conjecture for the density matrix of a finite segment of the XXZ chain coupled to a heat bath and to a constant longitudinal magnetic field. It states that the inhomogeneous density matrix, conceived as a map which associates with every local operator its thermal expectation value, can be written as the trace of the exponential of an operator constructed from weighted traces of the elements of certain monodromy matrices related to $U_q(\widehat{\mathfrak{sl}}_2)$ and only two transcendental functions pertaining to the one-point function and the neighbour correlators, respectively. Our conjecture implies that all static correlation functions of the XXZ chain are polynomials in these two functions and their derivatives with coefficients of purely algebraic origin.

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1. Introduction

The past two decades have seen significant progress in the understanding of the correlation functions of local operators in spin- $\frac{1}{2}$ chains. This report is about the extension of recent results for the ground-state correlators of the XXZ chain, surveyed below, to finite temperatures.

The development was initiated with the derivation of a multiple integral formula for the density matrix of the XXZ chain by the Kyoto school [24–26] which relies on the bosonization of q -vertex operators and on the q -Knizhnik–Zamolodchikov equation [18, 35]. An alternative derivation of the multiple integral formula was found in [29]. It is based on the algebraic Bethe ansatz and made it possible to include a longitudinal magnetic field.

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The multiple integral formulae, however, turned out to be numerically inefficient. They were hence not much used before it was realized [9] that they may be calculated by hand, at least in principle. This result generalized after many years Takahashi's curious formula [39] for the next-to-nearest neighbour correlator and inspired a series of works devoted to the explicit calculation of short-distance correlators in the XXX [10, 11, 15, 32–34] and XXZ chains [27, 28, 40]. It further triggered a deep investigation into the mathematical structure of the inhomogeneous density matrix of the XXZ chain, which was started in [12–14] and still continues [2–7].

In [2], a minimal set of equations that determines the inhomogeneous density matrix was derived and was termed the reduced q -Knizhnik–Zamolodchikov (rqKZ) equation. The rqKZ equation made it possible to prove that the correlation functions of the inhomogeneous XXX model depend on a single transcendental function which is basically the two-spinon scattering phase. This was generalized to the XXZ and XYZ models in [3, 7], where further transcendental functions were needed.

A new 'exponential form' of the density matrix was derived in [4, 5] for which the homogeneous (physical) limit can be taken directly. The most recent papers [6, 8] aimed at understanding how the exponential formula works in the 'free fermion' XX limit. This also led to a novel formulation for generic q . A crucial tool was a disorder field acting on half of the infinite lattice with 'strength' α . It regularized the problem further and simplified the exponential formula in a way that the exponent depends only on a single transcendental function ω and on special operators \mathbf{b} and \mathbf{c} resembling annihilation operators of (Dirac) fermions.

From the above studies we observe the following. In the inhomogeneous case, the multiple integrals reduce to polynomials in a small number of different single integrals related to the correlation functions of only nearest-neighbouring lattice sites. These constitute a set of transcendental functions which determine what we call the 'physical part' of the problem. The coefficients of the polynomials are rational functions of the inhomogeneity parameters. They are constructed from various L -operators related to the symmetry of the models and constitute the 'algebraic part'. We call such type of separation of the problem into a finite physical part and into an algebraic part 'factorization', since it can be traced back to the factorization of multiple integrals into single integrals. We believe that factorization is a general feature of integrable models (for a similar phenomenon in the form factors for the Ising model see [16]).

A generalization of the integral formula for the density matrix of the XXZ chain to finite temperature and magnetic field was derived in [19, 21, 22] by combining the techniques developed in [29] with the finite temperature formalism of [30, 31, 36–38]. Remarkably, the form of the multiple integrals for the density matrix elements is the same in all known cases. The physical parameters (temperature T , magnetic field h , chain length L) enter only indirectly through an auxiliary function which is defined as a solution of a nonlinear integral equation.

The auxiliary function enters into the multiple integrals as a weight function. This implies that the factorization technique developed for the ground-state correlators in [9] does not work any longer. In our previous work [1], we nevertheless obtained a factorization of the correlation functions of up to three neighbouring sites in the XXX model at arbitrary T, h by implicit use of a certain integral equation. Comparing the factorized forms with the known results for the ground state we could conjecture an exponential formula for the special case of $T > 0$ but $h = 0$. Surprisingly, the formula shares the same algebraic part with its $T = 0$ counterpart; one only has to replace the transcendental function by its finite temperature generalization. The results easily translated into similar results for the ground state of the system of finite length [17].

In this work, we extend our analysis to the periodic XXZ chain

$$\mathcal{H}_N = J \sum_{j=-N+1}^N (\sigma_{j-1}^x \sigma_j^x + \sigma_{j-1}^y \sigma_j^y + \Delta (\sigma_{j-1}^z \sigma_j^z - 1)) \quad (1)$$

in the antiferromagnetic regime ($J > 0$ and $\Delta = \text{ch}(\eta) > -1$) and in the thermodynamic limit ($L = 2N \rightarrow \infty$). We identify an appropriate set of basic functions describing the neighbour correlators in the inhomogeneous case. The algebraic part of the problem without magnetic field is neatly formulated in terms of the operators \mathbf{b} and \mathbf{c} as in the ground-state case. The meaning of the disorder parameter α , necessary for the construction of these operators, is yet to be understood for finite temperatures. It, however, naturally modifies one of our auxiliary functions, the density function G and allows us to reduce the number of basic functions characterizing the physical part from two to one.

Still, we go one important step further. We extend our conjectured exponential formula for the (finite temperature) density matrix such as to include the magnetic field. At first sight, this may seem to require only trivial modifications, as the Hamiltonian commutes with the Zeeman term. The magnetic field, however, breaks the $U_q(\widehat{\mathfrak{sl}}_2)$ symmetry and, as far as the factorization of the integrals is concerned, brings about serious difficulties even for the ground-state correlator problem. For this reason, an essential modification of the operator in the exponent of our exponential formula is required which leads to novel formulae even in the zero temperature limit. The prescription is, however, remarkably simple. We have to add a term whose algebraic part is determined by a new operator \mathbf{H} , such that the operator in the exponent is now a sum of two ingredients. One is formally identical to the operator already present at vanishing magnetic field, the other one is constructed from \mathbf{H} (note that even the former part is not independent of the field; it includes transcendental functions which are even functions of h).

We finally point out a simplification compared to the ground-state case, particularly relevant at finite magnetic field. Although we are dealing with highly non-trivial functions, all correlation functions should simplify in the vicinity of $T = \infty$. Thus, the high-temperature expansion technique can be applied to the multiple integral formulae at $T > 0$ as was shown in [41, 42]. We use this in order to test our conjecture for the exponential form of the density matrix.

Our paper is organized as follows. In section 2, we recall the definition of the density matrix and the multiple integral formulae. In section 3, we describe the basic functions that determine the physical part of the correlation functions. Our main result is presented in section 4 (see equations (36)–(38)). It is a conjectured exponential formula for the density matrix of the XXZ chain at finite temperature and magnetic field. Section 5 is devoted to the simplest examples of the correlation functions, the cases of $n = 1, 2, 3$, for which we show novel explicit formulae. In section 6, we summarize and discuss our results. Appendix A contains the proofs of two formulae needed in the main body of the paper, appendix B a derivation of the factorized form of the density matrix for $n = 2$ directly from the double integrals and appendix C a short description of the high-temperature expansion technique.

2. Multiple integral representation of the density matrix

Let us recall the definition of the density matrix of a chain segment of length n . We would like to take into account a longitudinal magnetic field h which couples to the conserved

z -component

$$S_N^z = \frac{1}{2} \sum_{j=-N+1}^N \sigma_j^z \quad (2)$$

of the total spin. Then, the statistical operator of the equilibrium system at temperature T is given by

$$\rho_N(T, h) = \frac{e^{-\frac{\mathcal{H}_N}{T} + \frac{hS_N^z}{T}}}{\text{tr}_{-N+1, \dots, N} e^{-\frac{\mathcal{H}_N}{T} + \frac{hS_N^z}{T}}}. \quad (3)$$

From this operator we obtain the density matrix of a chain segment of length n by tracing out the complementary degrees of freedom,

$$D_n(T, h|N) = \text{tr}_{-N+1, \dots, -1, 0, n+1, n+2, \dots, N} \rho_N(T, h), \quad n = 1, \dots, N. \quad (4)$$

The density matrix $D_n(T, h|N)$ encodes the complete equilibrium information about the segment consisting of sites $1, \dots, n$ which means that every operator \mathcal{O} acting non-trivially at most on sites $1, \dots, n$ has thermal expectation value

$$\langle \mathcal{O} \rangle_{T, h} = \text{tr}_{1, \dots, n} (D_n(T, h|N) \mathcal{O}). \quad (5)$$

We know a multiple integral representation for the density matrix (4) in two limiting cases, the thermodynamic limit $N \rightarrow \infty$ [19, 21] and the zero temperature and zero magnetic field limit [17]. For the two limits we shall employ the notation

$$D_n(T, h) = \lim_{N \rightarrow \infty} D_n(T, h|N), \quad D_n(N) = \lim_{T \rightarrow 0} \lim_{h \rightarrow 0} D_n(T, h|N). \quad (6)$$

These two density matrices are conveniently described in terms of the canonical basis of endomorphisms on $(\mathbb{C}^2)^{\otimes n}$ locally given by 2×2 matrices e_{β}^{α} , $\alpha, \beta = \pm$, with a single nonzero entry at the intersection of row β and column α ,

$$D_n(T, h) = D_{n\alpha_1, \dots, \alpha_n}^{\beta_1, \dots, \beta_n}(T, h) e_{\alpha_1}^{\beta_1} \dots e_{\alpha_n}^{\beta_n}, \quad D_n(N) = D_{n\alpha_1, \dots, \alpha_n}^{\beta_1, \dots, \beta_n}(N) e_{\alpha_1}^{\beta_1} \dots e_{\alpha_n}^{\beta_n}, \quad (7)$$

where we assume implicit summation over all $\alpha_j, \beta_k = \pm$. We further regularize the density matrices by introducing a set of parameters $\lambda_1, \dots, \lambda_n; \alpha$ in such a way that

$$D_n(T, h) = \lim_{\lambda_1, \dots, \lambda_n \rightarrow 0} \lim_{\alpha \rightarrow 0} D_{n\alpha_1, \dots, \alpha_n}^{\beta_1, \dots, \beta_n}(\lambda_1, \dots, \lambda_n | T, h; \alpha) e_{\alpha_1}^{\beta_1} \dots e_{\alpha_n}^{\beta_n}, \quad (8a)$$

$$D_n(N) = \lim_{\lambda_1, \dots, \lambda_n \rightarrow \eta/2} \lim_{\alpha \rightarrow 0} D_{n\alpha_1, \dots, \alpha_n}^{\beta_1, \dots, \beta_n}(\lambda_1, \dots, \lambda_n | N; \alpha) e_{\alpha_1}^{\beta_1} \dots e_{\alpha_n}^{\beta_n}. \quad (8b)$$

From here on we shall concentrate on the temperature case (8a). Later we will indicate the modifications necessary for (8b). We call $D_{n\alpha_1, \dots, \alpha_n}^{\beta_1, \dots, \beta_n}(\lambda_1, \dots, \lambda_n | T, h; \alpha)$ the inhomogeneous density matrix element with inhomogeneity parameters λ_j . For $\alpha = 0$ it has a clear interpretation in terms of the six-vertex model with spectral parameters $\lambda_1, \dots, \lambda_n$ on n consecutive vertical lines [22]. For $h, T = 0$ the variable α can be interpreted as a disorder parameter [25]. In the general case we simply define the inhomogeneous density matrix element by the following multiple integral:

$$\begin{aligned} & D_{n\alpha_1, \dots, \alpha_n}^{\beta_1, \dots, \beta_n}(\lambda_1, \dots, \lambda_n | T, h; \alpha) \\ &= \delta_{s, m-s'} \left[\prod_{j=1}^s \int_{\mathcal{C}} \frac{d\omega_j e^{-\alpha\eta}}{2\pi i (1 + \mathbf{a}(\omega_j))} \prod_{k=1}^{x_j-1} \text{sh}(\omega_j - \lambda_k - \eta) \prod_{k=x_j+1}^n \text{sh}(\omega_j - \lambda_k) \right] \\ & \times \left[\prod_{j=s+1}^n \int_{\mathcal{C}} \frac{d\omega_j e^{\alpha\eta}}{2\pi i (1 + \bar{\mathbf{a}}(\omega_j))} \prod_{k=1}^{x_j-1} \text{sh}(\omega_j - \lambda_k + \eta) \prod_{k=x_j+1}^n \text{sh}(\omega_j - \lambda_k) \right] \\ & \times \frac{\det[-G(\omega_j, \lambda_k; \alpha)]}{\prod_{1 \leq j < k \leq n} \text{sh}(\lambda_k - \lambda_j) \text{sh}(\omega_j - \omega_k - \eta)}. \end{aligned} \quad (9)$$

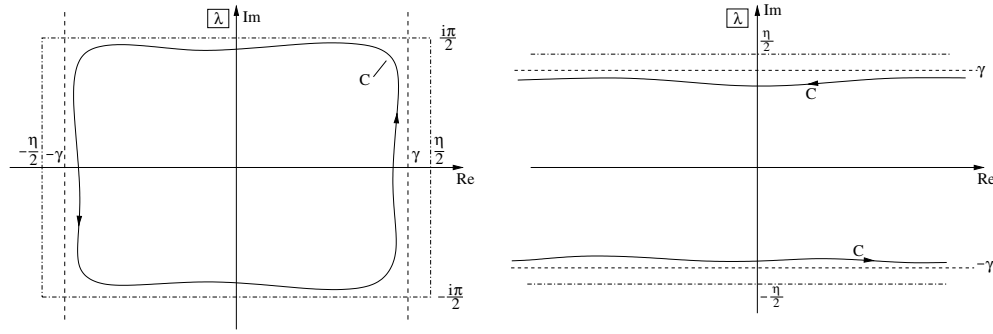


Figure 1. The canonical contour C for the off-critical regime $\Delta > 1$ (left) and for the critical regime $-1 < \Delta < 1$ (right).

Here, s is the number of plus signs in the sequence $(\alpha_j)_{j=1}^n$ and s' is the number of minus signs in the sequence $(\beta_j)_{j=1}^n$. The factor $\delta_{s,m-s'}$ reflects the conservation of the z -component of the total spin. For $j = 1, \dots, s$ the variable x_j denotes the position of the j th plus sign in $(\alpha_j)_{j=1}^n$ counted from the right. For $j = s+1, \dots, n$ it denotes the position of $(j-s)$ th minus sign in $(\beta_j)_{j=1}^n$. The integration contour depends on η . We show it in figure 1. This contour will also appear in the integral equations which determine the transcendental functions α , $\bar{\alpha}$ and G and in the definition of the special functions in the following section that determine the physical part in the factorized form of the correlation functions. For this reason, we call it the canonical contour.

The integral equation for α is nonlinear,

$$\ln \alpha(\lambda) = -\frac{h}{T} - \frac{2J \operatorname{sh}^2(\eta)}{T \operatorname{sh}(\lambda) \operatorname{sh}(\lambda + \eta)} - \int_C \frac{d\omega}{2\pi i} \frac{\operatorname{sh}(2\eta) \ln(1 + \alpha(\omega))}{\operatorname{sh}(\lambda - \omega + \eta) \operatorname{sh}(\lambda - \omega - \eta)}. \quad (10)$$

There is a similar integral equation for $\bar{\alpha}$ (see [20]); however, since $\bar{\alpha} = 1/\alpha$ we do not need to consider it here. α is usually called the auxiliary function. The combination $1/(1 + \alpha)$ has a natural interpretation as a generalization of the fermi function to the interacting case [23]. Note that the right-hand side of equation (10) is the only place where the thermodynamic variables T and h enter explicitly into our formulae for the correlation functions. They neither enter explicitly into the multiple integral formula (9) nor into the linear integral equation for G which is

$$G(\lambda, \mu; \alpha) = -\coth(\lambda - \mu) + e^{\alpha\eta} \coth(\lambda - \mu - \eta) + \int_C \frac{d\omega}{2\pi i} \frac{G(\omega, \mu; \alpha)}{1 + \alpha(\omega)} K(\lambda - \omega; \alpha). \quad (11)$$

G can be interpreted as a generalized magnetization density (see [20]). Compared to our previous definition [20] we introduced the additional parameter α here which also enters the kernel,

$$K(\lambda; \alpha) = e^{\alpha\eta} \coth(\lambda - \eta) - e^{-\alpha\eta} \coth(\lambda + \eta). \quad (12)$$

An equivalent integral equation for G which uses $\bar{\alpha}$ instead of α and which is sometimes useful is

$$G(\lambda, \mu; \alpha) = -\coth(\lambda - \mu) + e^{-\alpha\eta} \coth(\lambda - \mu + \eta) - \int_C \frac{d\omega}{2\pi i} \frac{G(\omega, \mu; \alpha)}{1 + \bar{\alpha}(\omega)} K(\lambda - \omega; \alpha). \quad (13)$$

Setting $\alpha = 0$ the function $G(\lambda, \mu; \alpha)$ turns into the function $G(\lambda, \mu)$ which played a crucial role in our previous studies [1, 20, 22]. We have introduced α in such a way into (9)

and (11) that for $T, h = 0$ the multiple integral representation (9) turns into the finite- α expression that can be obtained within the q -vertex operator approach of [25]. Our main motivation for introducing α into our functions was to enforce compatibility with the formalism developed in [6], where α is an important regularization parameter. The usefulness of this modification will become clear in section 4. The parameter α will allow us to write our formula for the density matrix in factorized form in a very compact way.

Let us briefly indicate the changes that are necessary in the finite length case (8b). It turns out [17] that $D_{n\alpha_1, \dots, \alpha_n}^{\beta_1, \dots, \beta_n}(\lambda_1, \dots, \lambda_n | N; \alpha)$ has a multiple integral representation of the same form as (9), that even the integral equation for G remains the same and that the only necessary modification is in the driving term of the nonlinear integral equation (10), where the physical parameters enter, which in this case are the length $L = 2N$ of the chain and an arbitrary twist $\Phi \in [0, 2\pi)$ of the periodic boundary conditions (for details see [17]). The nonlinear integral equation for the finite length case is

$$\ln \alpha(\lambda) = -2i\Phi + L\eta + L \ln \left(\frac{\text{sh}(\lambda - \frac{\eta}{2})}{\text{sh}(\lambda + \frac{\eta}{2})} \right) - \int_{\mathcal{C}} \frac{d\omega}{2\pi i} \frac{\text{sh}(2\eta) \ln(1 + \alpha(\omega))}{\text{sh}(\lambda - \omega + \eta) \text{sh}(\lambda - \omega - \eta)}. \quad (14)$$

When we derived the multiple integral representation (9) in [17, 19] we assumed that the inhomogeneity parameters λ_j are located inside the integration contour \mathcal{C} . This has to be taken into account when calculating the homogeneous limit in (8b), where the canonical contour should be first shifted to $\pm\eta/2$.

3. The basic functions

In this section, we describe the functions constituting the ‘physical part’ of the factorized correlation functions of the XXZ chain at finite T and h . A description of the algebraic part will be given in the next section. According to our experience, the physical part of the correlation functions can be characterized completely by two transcendental functions φ and ω .

Let us start with the more simple function

$$\varphi(\mu; \alpha) = 1 + \int_{\mathcal{C}} \frac{d\omega G(\omega, \mu; \alpha)}{\pi i (1 + \alpha(\omega))}. \quad (15)$$

This function is related to the magnetization $m(T, h)$ through $\varphi(0; 0) = -2m(T, h)$ which we expect to belong to the physical part if the magnetic field is nonzero.

In order to introduce the function ω we first of all define

$$\psi(\mu_1, \mu_2; \alpha) = \int_{\mathcal{C}} \frac{d\omega G(\omega, \mu_1; \alpha)}{\pi i (1 + \alpha(\omega))} (-\coth(\omega - \mu_2) + e^{-\alpha\eta} \coth(\omega - \mu_2 - \eta)). \quad (16)$$

Those readers who are familiar with our previous work [1] will recognize this as the anisotropic and ‘ α -deformed’ version of the function $\psi(\mu_1, \mu_2)$ introduced there. The function ω is a modification of ψ obtained by adding and multiplying some explicit functions:

$$\omega(\mu_1, \mu_2; \alpha) = -e^{\alpha(\mu_1 - \mu_2)} \psi(\mu_1, \mu_2; \alpha) - \frac{e^{\alpha(\mu_1 - \mu_2)}}{2 \cosh^2(\frac{\alpha\eta}{2})} K(\mu_1 - \mu_2; -\alpha). \quad (17)$$

Here $K(\lambda; \alpha)$ is the kernel defined in (12). The relation between $\omega(\mu_1, \mu_2; \alpha)$ and $\psi(\mu_1, \mu_2; \alpha)$ is similar to the relation between $\gamma(\mu_1, \mu_2)$ and $\psi(\mu_1, \mu_2)$ in the isotropic case [1]. The function ω is closely related to the neighbour correlators (see appendix B). In the critical regime for $T, h \rightarrow 0$ it becomes the function $\omega(\zeta, \alpha)$ of the paper [6] if we set $\zeta = e^{\mu_1 - \mu_2}$.

An important property which follows from the definitions (12) and (16) is that

$$\omega(\mu_2, \mu_1; -\alpha) = \omega(\mu_1, \mu_2; \alpha). \quad (18)$$

It implies

$$\omega(\mu_2, \mu_1; 0) = \omega(\mu_1, \mu_2; 0), \quad \omega'(\mu_2, \mu_1; 0) = -\omega'(\mu_1, \mu_2; 0), \quad (19)$$

where for later convenience we introduced the somewhat unusual notation

$$\omega'(\mu_1, \mu_2; \alpha) = \partial_\alpha (e^{\alpha(\mu_2 - \mu_1)} \omega(\mu_1, \mu_2; \alpha)). \quad (20)$$

At this point we would like to stress that the physical parameters T , h or N , respectively, do not enter the definitions of φ and ω explicitly. The basic functions defined in this section are therefore suitable for both the finite temperature and the finite length case, the only distinction being the use of different auxiliary function (10) and (14), respectively.

In the high-temperature limit (see appendix C) we observe that

$$\omega(\mu_1, \mu_2; \alpha) = \frac{e^{\alpha(\mu_1 - \mu_2)}}{2} \tanh^2\left(\frac{\alpha\eta}{2}\right) K(\mu_1 - \mu_2; -\alpha) + \mathcal{O}\left(\frac{1}{T}\right). \quad (21)$$

Using equation (21) we conclude that both functions $\omega(\mu_1, \mu_2; 0)$ and $\omega'(\mu_1, \mu_2; 0)$ do not have zeroth-order terms in their high-temperature expansions

$$\omega(\mu_1, \mu_2; 0) = \mathcal{O}(1/T), \quad \omega'(\mu_1, \mu_2; 0) = \mathcal{O}(1/T). \quad (22)$$

The same is true for the function φ ,

$$\varphi(\mu; \alpha) = \mathcal{O}(1/T). \quad (23)$$

We mention the properties of these functions for $\alpha = 0$ with respect to reversal of the magnetic field; $\varphi(\mu; 0)$ is an odd function of h , $\psi(\mu_1, \mu_2; 0)$ and $\partial_\alpha \psi(\mu_1, \mu_2; \alpha)|_{\alpha=0}$ are even. These properties will be implicitly used below. The proof relies on the simple fact that the quantum transfer matrix (or its slight generalization, see below) associated with the present model respects the spin reversal symmetry, and therefore the eigenvalues are even functions of h .

Once this is realized, the proof for $\varphi(\mu; 0)$ is rather obvious. One only has to remember the relation between $\varphi(\mu; 0)$ and the largest eigenvalue $\Lambda(\mu)$ of the quantum transfer matrix,

$$\varphi(\mu; 0) = T \frac{\partial}{\partial h} \ln \Lambda(\mu). \quad (24)$$

The above argument then implies that $\varphi(\mu; 0)$ is odd with respect to h .

The proof for $\psi(\mu_1, \mu_2; 0)$ is less obvious. We first of all introduce a generalized system. Consider an ‘alternating’ inhomogeneous transfer matrix. In the framework of the quantum transfer matrix, we associate spectral parameters in alternating manner ($u, -u, u, -u \dots$) to $2\mathcal{N}$ vertical bonds, while keeping the spectral parameter on the horizontal axis fixed as μ_2 . Next we add $2\mathcal{M}$ vertical bonds and associate with them spectral parameters again in alternating manner, ($u' + \mu_1, \mu_1 - u', u' + \mu_1, \mu_1 - u', \dots$). We then take the limit $\mathcal{N}, \mathcal{M} \rightarrow \infty$ under the fine tuning, $2u\mathcal{N} = 2\beta J \operatorname{sh} \eta$, $2u'\mathcal{M} = -2\delta J \operatorname{sh} \eta$. Note that the original system is recovered by taking $\delta = 0$. By neglecting the term depending on the overall normalization, one obtains the following expression for the modified largest eigenvalue $\Lambda(\mu_2, \mu_1)$ of the generalized quantum transfer matrix:

$$\ln \Lambda(\mu_2, \mu_1) = -\frac{\beta h}{2} - \int_{\mathcal{C}} \frac{d\omega}{2\pi i} e(\omega - \mu_2) \ln(1 + \bar{a}(\omega, \mu_1)), \quad e(\lambda) := \frac{\operatorname{sh}(\eta)}{\operatorname{sh}(\lambda) \operatorname{sh}(\lambda - \eta)}. \quad (25)$$

The modified auxiliary functions $a(\omega, \mu_1)$, $\bar{a}(\omega, \mu_1)$ satisfy equations similar to (10), and the equation for the latter is relevant here:

$$\begin{aligned} \ln \bar{a}(\lambda, \mu_1) &= \frac{h}{T} - \frac{2J \operatorname{sh}(\eta)}{T} e(\lambda) + 2\delta J \operatorname{sh}(\eta) e(\lambda - \mu_1) \\ &+ \int_{\mathcal{C}} \frac{d\omega}{2\pi i} K(\lambda - \omega; 0) \ln(1 + \bar{a}(\omega, \mu_1)). \end{aligned} \quad (26)$$

We take the derivative of both sides of (26) with respect to δ ,

$$\sigma(\lambda, \mu_1) = 2J \operatorname{sh}(\eta) e(\lambda - \mu_1) + \int_C \frac{d\omega}{2\pi i} K(\lambda - \omega; 0) \frac{\sigma(\omega, \mu_1)}{(1 + \mathfrak{a}(\omega, \mu_1))}, \quad (27)$$

where $\sigma(\lambda, \mu_1) := \frac{1}{\bar{\mathfrak{a}}(\lambda, \mu_1)} \frac{\partial}{\partial \delta} \bar{\mathfrak{a}}(\lambda, \mu_1)$. One compares (11) with (26) and concludes

$$\sigma(\lambda, \mu_1) = 2J \operatorname{sh}(\eta) G(\lambda, \mu_1; 0). \quad (28)$$

Similarly, we take the derivative of $\ln \Lambda(\mu_2, \mu_1)$ with respect to δ and find

$$\begin{aligned} \frac{\partial}{\partial \delta} \ln \Lambda(\mu_2, \mu_1) &= - \int_C \frac{d\omega}{2\pi i} e(\omega - \mu_2) \frac{\sigma(\omega, \mu_1)}{(1 + \mathfrak{a}(\omega, \mu_1))} \\ &= - \int_C \frac{d\omega}{2\pi i} e(\omega - \mu_2) \frac{2J \operatorname{sh}(\eta) G(\omega, \mu_1; 0)}{(1 + \mathfrak{a}(\omega, \mu_1))} \\ &= -J \operatorname{sh}(\eta) \int_C \frac{d\omega}{\pi i} \frac{G(\omega, \mu_1; 0)}{(1 + \mathfrak{a}(\omega, \mu_1))} (\coth(\omega - \mu_2 - \eta) - \coth(\omega - \mu_2)), \end{aligned} \quad (29)$$

where we have used (28) in the second equality. By comparing the above equation with (16), one obtains

$$\psi(\mu_1, \mu_2; 0) = \frac{1}{J \operatorname{sh}(\eta)} \frac{\partial}{\partial \delta} \ln \Lambda(\mu_2, \mu_1)|_{\delta=0}. \quad (30)$$

Then, the evenness of $\psi(\mu_1, \mu_2; 0)$ follows from the same property of the generalized transfer matrix.

Finally, we show that $\partial_\alpha \psi(\lambda_1, \lambda_2; \alpha)|_{\alpha=0}$ is also even. To prove this we consider relation (B.5) in appendix B. The lhs, $D_{-+}^+(\lambda_1, \lambda_2) + D_{+-}^+(\lambda_1, \lambda_2)$, is invariant under $+ \leftrightarrow -$; hence, it is even with respect to h . The first term in the rhs is also even as it is proportional to $\psi(\mu_1, \mu_2; 0)$ (see (B.11)). Thus, the content of the bracket in the second term of the rhs should also be even. Thanks to (B.3) and (B.17) it is represented as

$$\begin{aligned} D_+^+(\lambda_1) + D_+^+(\lambda_2) - 2D_{++}^+(\lambda_1, \lambda_2) &= \frac{\coth(\eta)}{2} \psi(\lambda_1, \lambda_2; 0) \\ &+ \frac{\coth(\lambda_1 - \lambda_2)}{2\eta} \partial_\alpha \psi(\lambda_1, \lambda_2; \alpha)|_{\alpha=0}. \end{aligned}$$

Thus, we conclude that $\partial_\alpha \psi(\lambda_1, \lambda_2; \alpha)|_{\alpha=0}$ is even.

4. Thermal correlation functions of local operators

In this section, we are formulating our main result which is a conjectured explicit formula for the correlation functions of local operators in the XXZ chain at finite temperature and finite magnetic field. The sources of this conjecture are the results of the previous two sections that followed from the finite temperature algebraic Bethe ansatz approach of [17, 20, 22] and the results of [4, 6, 7], where the exponential formula was discovered as a consequence of studying the rqKZ equation. Unfortunately, both approaches differ considerably in spirit and notation. We will try to reconcile them while keeping as much as possible of the original notation. We have to ask the reader to be forbearing though if this sometimes leads to confusion.

In [6], much emphasis was laid on developing a formalism which applies directly to the infinite chain with lattice sites $j \in \mathbb{Z}$. To keep things closely parallel we therefore concentrate in this section on the temperature case and comment on the finite length case only later in section 6. All operators \mathcal{O} which act non-trivially on any finite number of lattice sites span a vector space \mathcal{W} . Because of the translational invariance of the Hamiltonian we may content ourselves (as long as we keep $\alpha = 0$) with operators which act non-trivially only on positive

lattice sites, $j \in \mathbb{N}$. We shall denote the restriction of \mathcal{O} to the first n lattice sites by $\mathcal{O}_{[1,n]}$. The inhomogeneous density matrix satisfies the reduction identity

$$\mathrm{tr}_n D_n(\lambda_1, \dots, \lambda_n | T, h; 0) = D_{n-1}(\lambda_1, \dots, \lambda_{n-1} | T, h; 0). \quad (31)$$

It follows that the inductive limit

$$\lim_{n \rightarrow \infty} \mathrm{tr}_{1, \dots, n} (D_n(\lambda_1, \dots, \lambda_n | T, h; 0) \mathcal{O}_{[1,n]}) \quad (32)$$

exists and defines an operator $D_{T,h}^* : \mathcal{W} \rightarrow \mathbb{C}$ such that

$$D_{T,h}^*(\mathcal{O}) = \langle \mathcal{O} \rangle_{T,h} \quad (33)$$

is the thermal average at finite magnetic field of the local operator \mathcal{O} in the inhomogeneous XXZ model. Note that

$$D_{T,h}^*(e_{1\beta_1}^{\alpha_1} \dots e_{n\beta_n}^{\alpha_n}) = D_{n\alpha_1, \dots, \alpha_n}^{\beta_1, \dots, \beta_n}(\lambda_1, \dots, \lambda_n | T, h; 0). \quad (34)$$

For this reason we may interpret $D_{T,h}^*$ as a kind of ‘universal density matrix’ of the XXZ chain.

Let us define a linear functional $\mathbf{tr} : \mathcal{W} \rightarrow \mathbb{C}$ by

$$\mathbf{tr}(\mathcal{O}) = \dots \frac{1}{2} \mathrm{tr}_1 \frac{1}{2} \mathrm{tr}_2 \frac{1}{2} \mathrm{tr}_3 \dots (\mathcal{O}), \quad (35)$$

with tr_j being the usual traces of 2×2 matrices. Then we conjecture that an operator $\Omega : \mathcal{W} \rightarrow \mathcal{W}$ exists such that $D_{T,h}^* = \mathbf{tr} e^\Omega$. More precisely we propose the following.

Conjecture. For all $\mathcal{O} \in \mathcal{W}$ the density matrix $D_{T,h}^*$ can be expressed as

$$D_{T,h}^*(\mathcal{O}) = \mathbf{tr}(e^\Omega(\mathcal{O})), \quad (36)$$

where \mathbf{tr} is the trace functional (35) and $\Omega : \mathcal{W} \rightarrow \mathcal{W}$ is a linear operator that can be decomposed as

$$\Omega = \Omega_1 + \Omega_2 \quad (37)$$

with

$$\Omega_1 = - \lim_{\alpha \rightarrow 0} \int \frac{d\mu_1}{2\pi i} \frac{d\mu_2}{2\pi i} \omega(\mu_1, \mu_2; \alpha) \mathbf{b}(\zeta_1; \alpha - 1) \mathbf{c}(\zeta_2; \alpha), \quad (38a)$$

$$\Omega_2 = - \lim_{\alpha \rightarrow 0} \int \frac{d\mu_1}{2\pi i} \varphi(\mu_1; \alpha) \mathbf{H}(\zeta_1; \alpha). \quad (38b)$$

Here $\zeta_j = e^{\mu_j}$, $j = 1, 2$, and $\omega(\mu_1, \mu_2; \alpha)$ and $\varphi(\mu_1; \alpha)$ are the functions defined in (17) and (15). The operators \mathbf{b} , \mathbf{c} and \mathbf{H} do not depend on T or h . They are purely algebraic. Their construction will be explained below. The integrals mean to take residues at the simple poles of \mathbf{b} , \mathbf{c} and \mathbf{H} located at the inhomogeneities ξ_j (see below).

In fact, the operators \mathbf{b} and \mathbf{c} are the same as in the ground-state case [6]. The operator \mathbf{H} is new in the present context⁴, but can be defined using the same algebraic notions underlying the construction of \mathbf{b} and \mathbf{c} . Note that $\lim_{h \rightarrow 0} \varphi(\mu; 0) = 0$ which implies that $\lim_{h \rightarrow 0} \Omega_2 = 0$. Hence, as in the isotropic case [1], we observe that the algebraic structure of the factorized form of the correlation functions is identical in the ground state and for finite temperature as long as the magnetic field vanishes. Due to the properties of the function ω we recover the result of [6] in the zero temperature limit at vanishing magnetic field. In the high-temperature limit, on the other hand, we conclude with (22) and (23) that $\lim_{T \rightarrow \infty} \Omega = 0$ and that all correlation functions trivialize in the expected way:

$$\lim_{T \rightarrow \infty} D_{T,h}^* = \mathbf{tr}. \quad (39)$$

⁴ Compare, however, equation (68) with the operator $\mathbf{k}^{(0)}$ defined in lemma A.2 of [8].

For the definition of the operators \mathbf{b} , \mathbf{c} and \mathbf{H} we first of all generalize the space of local operators \mathcal{W} to a space of quasi-local operators of the form

$$e^{\alpha\eta \sum_{k=-\infty}^0 \sigma_k^z} \mathcal{O}, \tag{40}$$

where \mathcal{O} is local and denote this space by \mathcal{W}_α . The operators \mathbf{b} , \mathbf{c} and \mathbf{H} then act as

$$\mathbf{b}(\zeta; \alpha) : \mathcal{W}_\alpha \rightarrow \mathcal{W}_{\alpha+1}, \quad \mathbf{c}(\zeta; \alpha) : \mathcal{W}_\alpha \rightarrow \mathcal{W}_{\alpha-1}, \quad \mathbf{H}(\zeta; \alpha) : \mathcal{W}_\alpha \rightarrow \mathcal{W}_\alpha \tag{41}$$

which implies in particular that $\mathbf{b}(\zeta_1; \alpha - 1)\mathbf{c}(\zeta_2; \alpha) : \mathcal{W}_\alpha \rightarrow \mathcal{W}_\alpha$.

The z -component of the total spin is the formal series S_∞^z (see equation (2)). We denote its adjoint action by

$$\mathbb{S}(X) = [S_\infty^z, X]. \tag{42}$$

Then $q^{\alpha S} : \mathcal{W}_\alpha \rightarrow \mathcal{W}_\alpha$. The spin reversal operator defined by

$$\mathbb{J}(X) = \left[\prod_{j \in \mathbb{Z}} \sigma_j^x \right] X \left[\prod_{j \in \mathbb{Z}} \sigma_j^x \right] \tag{43}$$

clearly is a map $\mathbb{J} : \mathcal{W}_\alpha \rightarrow \mathcal{W}_{-\alpha}$.

The operators \mathbf{b} , \mathbf{c} and \mathbf{H} will be defined in two steps. We first define endomorphisms $\mathbf{b}_{[kl]}$, $\mathbf{c}_{[kl]}$ and $\mathbf{H}_{[kl]}$ acting on $\text{End}(\mathcal{V})$, where the tensor product $\mathcal{V} = V_k \otimes \dots \otimes V_l$ represents the space of states of a segment of the infinite spin chain reaching from site k to site l , and V_j is isomorphic to \mathbb{C}^2 . Then we use that these endomorphisms have a reduction property similar to (31) which allows us to extend their action to \mathcal{W}_α by an inductive limit procedure. The endomorphisms $\mathbf{b}_{[kl]}$, $\mathbf{c}_{[kl]}$ and $\mathbf{H}_{[kl]}$ are constructed from weighted traces of the elements of certain monodromy matrices related to $U_q(\widehat{\mathfrak{sl}}_2)$. These monodromy matrices are obtained from products of L -matrices with different auxiliary spaces.

The simplest case is directly related to the R -matrix of the six-vertex model,

$$R(\zeta) = (q\zeta - q^{-1}\zeta^{-1}) \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \beta(\zeta) & \gamma(\zeta) & 0 \\ 0 & \gamma(\zeta) & \beta(\zeta) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{44}$$

where

$$\beta(\zeta) = \frac{(1 - \zeta^2)q}{1 - q^2\zeta^2}, \quad \gamma(\zeta) = \frac{(1 - q^2)\zeta}{1 - q^2\zeta^2} \tag{45}$$

and $q = e^{\alpha\eta}$. Let us fix an auxiliary space V_a isomorphic to \mathbb{C}^2 . Then $L_{a,j}(\zeta) = R_{a,j}(\zeta)$ is the standard L -matrix of the six-vertex model. The corresponding monodromy matrix is

$$T_{a,[k,l]}(\zeta) = L_{a,k}(\zeta/\xi_k) \cdots L_{a,l}(\zeta/\xi_l). \tag{46}$$

It acts on $V_a \otimes \mathcal{V}$. We are interested in operators acting on $\text{End}(\mathcal{V})$. Such type of operators are naturally given by the adjoint action of operators acting on \mathcal{V} . An example is the transfer matrix $\mathbf{t}_{[k,l]}(\zeta)$ defined by

$$\mathbf{t}_{[k,l]}(\zeta)(X) = \text{tr}_a T_{a,[k,l]}(\zeta)^{-1} X T_{a,[k,l]}(\zeta) \tag{47}$$

for all $X \in \text{End}(\mathcal{V})$. It will be needed in the definition of the operator $\mathbf{H}_{[k,l]}$ below.

Further following [6] we introduce another type of monodromy matrices for which the auxiliary space is replaced with the q -oscillator algebra Osc generated by $a, a^*, q^{\pm D}$ modulo the relations

$$\begin{aligned} q^D a^* &= a^* q^{D+1}, & q^D a &= a q^{D-1}, \\ a^* a &= 1 - q^{2D}, & a a^* &= 1 - q^{2D+2}. \end{aligned} \tag{48}$$

We consider two irreducible modules W^\pm of Osc ,

$$W^+ = \bigoplus_{k \geq 0} \mathbb{C}|k\rangle, \quad W^- = \bigoplus_{k \leq -1} \mathbb{C}|k\rangle, \quad (49)$$

defined by the action

$$q^D |k\rangle = q^k |k\rangle, \quad a|k\rangle = (1 - q^{2k})|k - 1\rangle, \quad a^*|k\rangle = (1 - \delta_{k,-1})|k + 1\rangle \quad (50)$$

of the generators. The L -operators $L^\pm(\zeta) \in \text{Osc} \otimes \text{End}(\mathcal{V})$ are defined by

$$L^+(\zeta) = i\zeta^{-1/2} q^{-1/4} (1 - \zeta a^* \sigma^+ - \zeta a \sigma^- - \zeta^2 q^{2D+2} \sigma^- \sigma^+) q^{\sigma^z D}, \quad (51a)$$

$$L^-(\zeta) = \sigma^x L^+(\zeta) \sigma^x. \quad (51b)$$

The corresponding monodromy matrices are

$$T_{A,[k,l]}^\pm(\zeta) = L_{A,l}^\pm(\zeta/\xi_l) \cdots L_{A,k}^\pm(\zeta/\xi_k), \quad (52)$$

where the index A refers to the auxiliary space Osc . We denote their (inverse) adjoint action by

$$\mathbb{T}_{A,[k,l]}^\pm(\zeta)^{-1}(X) = T_{A,[k,l]}^\pm(\zeta)^{-1} X T_{A,[k,l]}^\pm(\zeta) \quad (53)$$

for all $X \in \text{End}(\mathcal{V})$. Here, the inverse on the right-hand side is taken for both auxiliary and ‘quantum’ spaces. The analogue of the transfer matrix $\mathbf{t}_{[k,l]}$ in this case are two Q -operators Q^\pm (see [6]). Since we need only one of them here we leave out the superscript and define⁵

$$\mathbf{Q}_{[k,l]}(\zeta, \alpha) = \text{tr}_A^+ (q^{2\alpha D_A} \mathbb{T}_{A,[k,l]}^+(\zeta)^{-1}). \quad (54)$$

Here tr_A^+ signifies that the trace is taken over W^+ . Similarly, we will denote the trace over W^- by tr_A^- .

Now we are prepared to define the restriction of the operator \mathbf{H} to $\text{End}(\mathcal{V})$,

$$\mathbf{H}_{[k,l]}(\zeta; \alpha) = \mathbf{Q}_{[k,l]}(\zeta; \alpha) \mathbf{t}_{[k,l]}(\zeta). \quad (55)$$

We show below that this definition (in the limit $\alpha \rightarrow 0$) can be inductively extended to \mathcal{W}_α . To avoid possible confusion let us note that in fact the operator \mathbf{H} defined by formula (55) is *not* the left-hand side of Baxter’s TQ -relation. In order that it were we would need to ‘ α -deform’ the \mathbf{t} -operator as well.

In order to obtain $\mathbf{b}_{[k,l]}$ and $\mathbf{c}_{[k,l]}$ and also another form of the operator $\mathbf{H}_{[k,l]}$ we recall the fusion technique used in [6]. There the fused L -operators

$$L_{\{A,a\},j}^\pm(\zeta) = (G_{A,a}^\pm)^{-1} L_{A,j}^\pm(\zeta) R_{a,j}(\zeta) G_{A,a}^\pm \quad (56)$$

were defined, where

$$G_{A,a}^\pm = q^{\mp \sigma_a^z D_A} (1 + a_a^* \sigma^\pm). \quad (57)$$

The application of $G_{A,a}^+$ transforms $L_{A,j}^\pm(\zeta) R_{a,j}(\zeta)$ into a matrix of lower triangular form on V_a ,

$$L_{\{A,a\},j}^+(\zeta) = (\zeta q - \zeta^{-1} q^{-1}) \begin{pmatrix} L_{A,j}^+(q^{-1}\zeta) q^{-\sigma_j^z/2} & 0 \\ \gamma(\zeta) L_{A,j}^+(q\zeta) \sigma_j^+ q^{-2D_A+1/2} & \beta(\zeta) L_{A,j}^+(q\zeta) q^{\sigma_j^z/2} \end{pmatrix}_a. \quad (58)$$

⁵ Here, we use a slightly different definition of Q -operator in comparison with \mathbf{Q}^+ in [6], see formula (2.10) there. The difference is an additional factor $(1 - q^{2(\alpha-\bar{S})})$.

The inverse is also of lower triangular form and is given by

$$L_{\{A,a\},j}^+(\zeta)^{-1} = \frac{1}{q\zeta - q^{-1}\zeta^{-1}} \times \begin{pmatrix} q^{\sigma_j^z/2} L_{A,j}^+(q^{-1}\zeta)^{-1} & 0 \\ -\gamma(q^{-1}\zeta)\sigma_j^+ q^{-2D_A-1/2} L_{A,j}^+(q^{-1}\zeta)^{-1} & \beta(\zeta)^{-1} q^{-\sigma_j^z/2} L_{A,j}^+(q\zeta)^{-1} \end{pmatrix}_a. \quad (59)$$

Correspondingly

$$L_{\{A,a\},j}^-(\zeta) = \sigma_a^x \sigma_j^x L_{\{A,a\},j}^+(\zeta) \sigma_a^x \sigma_j^x \quad (60)$$

is of upper triangular form. It follows that similar statements hold for the monodromy matrices

$$T_{\{A,a\},[k,l]}^\pm(\zeta) = (G_{A,a}^\pm)^{-1} T_{A,[k,l]}^\pm(\zeta) T_{a,[k,l]}(\zeta) G_{A,a}^\pm. \quad (61)$$

$T_{\{A,a\},[k,l]}^+(\zeta)$ acts as a lower triangular matrix in V_a , $T_{\{A,a\},[k,l]}^-(\zeta)$ as an upper triangular matrix. As before we are interested in the adjoint action of the fused monodromy matrices on endomorphisms $X \in \text{End}(\mathcal{V})$. Following [6] we define

$$\mathbb{T}_{\{A,a\},[k,l]}^\pm(\zeta)^{-1}(X) = T_{\{A,a\},[k,l]}^\pm(\zeta)^{-1} X T_{\{A,a\},[k,l]}^\pm(\zeta) \quad (62)$$

for all $X \in \text{End}(\mathcal{V})$.

Regarding $\mathbb{T}_{\{A,a\},[k,l]}^\pm(\zeta)^{-1}$ as matrices acting on V_a as in [6] we may write their entries as

$$\begin{aligned} \mathbb{T}_{\{A,a\},[k,l]}^+(\zeta)^{-1} &= \begin{pmatrix} \mathbb{A}_{A,[k,l]}^+(\zeta) & 0 \\ \mathbb{C}_{A,[k,l]}^+(\zeta) & \mathbb{D}_{A,[k,l]}^+(\zeta) \end{pmatrix}_a, \\ \mathbb{T}_{\{A,a\},[k,l]}^-(\zeta)^{-1} &= \begin{pmatrix} \mathbb{A}_{A,[k,l]}^-(\zeta) & \mathbb{B}_{A,[k,l]}^-(\zeta) \\ 0 & \mathbb{D}_{A,[k,l]}^-(\zeta) \end{pmatrix}_a. \end{aligned} \quad (63)$$

The entries of these matrices are elements of $\text{Osc} \otimes \text{End}(\mathcal{V})$. We are now prepared to define $\mathbf{b}_{[k,l]}$ and $\mathbf{c}_{[k,l]}$,

$$\mathbf{c}_{[k,l]}(\zeta, \alpha) = q^{\alpha - \mathbb{S}_{[k,l]}} (1 - q^{2(\alpha - \mathbb{S}_{[k,l]})}) \text{sing}[\zeta^{\alpha - \mathbb{S}_{[k,l]}} \text{tr}_A^+(q^{2\alpha D_A} \mathbb{C}_{A,[k,l]}^+(\zeta))], \quad (64a)$$

$$\mathbf{b}_{[k,l]}(\zeta, \alpha) = q^{2\mathbb{S}_{[k,l]}} \text{sing}[\zeta^{-\alpha + \mathbb{S}_{[k,l]}} \text{tr}_A^-(q^{-2\alpha(D_A+1)} \mathbb{B}_{A,[k,l]}^-(\zeta))]. \quad (64b)$$

The symbol ‘sing’ means taking the singular part at $\zeta = \xi_j$, $j = 1, \dots, n$ (cf equation (2.13) of [6]). These operators raise or lower the z -component of the total spin by one,

$$[\mathbb{S}_{[k,l]}, \mathbf{c}_{[k,l]}(\zeta, \alpha)] = \mathbf{c}_{[k,l]}(\zeta, \alpha), \quad [\mathbb{S}_{[k,l]}, \mathbf{b}_{[k,l]}(\zeta, \alpha)] = -\mathbf{b}_{[k,l]}(\zeta, \alpha). \quad (65)$$

Their properties were extensively studied in [6, 8]. Here we shall only need the following.

Proposition 1. *Reduction properties [6]:*

$$\begin{aligned} \mathbf{c}_{[k,l]}(\zeta, \alpha)(X_{[k,l-1]} I_l) &= \mathbf{c}_{[k,l-1]}(\zeta, \alpha)(X_{[k,l-1]} I_l), \\ \mathbf{b}_{[k,l]}(\zeta, \alpha)(X_{[k,l-1]} I_l) &= \mathbf{b}_{[k,l-1]}(\zeta, \alpha)(X_{[k,l-1]} I_l), \\ \mathbf{c}_{[k,l]}(\zeta, \alpha)(q^{\alpha \sigma_k^z} X_{[k+1,l]}) &= q^{(\alpha-1)\sigma_k^z} \mathbf{c}_{[k+1,l]}(\zeta, \alpha)(X_{[k+1,l]}), \\ \mathbf{b}_{[k,l]}(\zeta, \alpha)(q^{\alpha \sigma_k^z} X_{[k+1,l]}) &= q^{(\alpha+1)\sigma_k^z} \mathbf{b}_{[k+1,l]}(\zeta, \alpha)(X_{[k+1,l]}). \end{aligned} \quad (66)$$

From this it follows that $\mathbf{c}_{[k,l]}(\zeta, \alpha)$ can be inductively extended to an operator $\mathbf{c}(\zeta, \alpha) : \mathcal{W}_\alpha \rightarrow \mathcal{W}_{\alpha-1}$. Similarly $\mathbf{b}_{[k,l]}(\zeta, \alpha)$ inductively extends to an operator $\mathbf{b}(\zeta, \alpha) : \mathcal{W}_\alpha \rightarrow \mathcal{W}_{\alpha+1}$. These are the operators appearing in the definition (38a) of Ω_1 .

Using the simple relation

$$(G_{A,a}^+)^{-1} q^{2\alpha D_A} G_{A,a}^+ = q^{2\alpha D_A} \begin{pmatrix} 1 & (1 - q^{-2\alpha}) a_A^* \\ 0 & 1 \end{pmatrix}_a \quad (67)$$

and the concrete form of $L_{[A,a],j}^+(\zeta)$ and $L_{[A,a],j}^+(\zeta)^{-1}$ one can obtain

$$\mathbf{H}_{[k,l]}(\zeta; \alpha) \simeq (1 - q^{-2\alpha}) \text{tr}_A^+ (q^{2\alpha D_A} a_A^* \mathbb{C}_{A,[k,l]}^+(\zeta)), \quad (68)$$

where the symbol \simeq means equality up to the regular part when $\zeta \rightarrow \xi_j$. Since the function $\varphi(\mu, \alpha)$ is regular when $\mu \rightarrow 0$, the regular part of $\mathbf{H}_{[k,l]}(\zeta; \alpha)$ does not contribute to the right-hand side of (38b). Formula (68) looks rather similar to the definition (64a) of the operator $\mathbf{c}_{[k,l]}$. The essential difference is due to the insertion of a_A^* under the trace. In contrast to the $\mathbf{c}_{[k,l]}$ -operator which increases the total spin, the operator $\mathbf{H}_{[k,l]}$ does not change the total spin.

4.1. Properties of the operators Ω_1 and Ω_2

Assuming for a moment that the limit on the right-hand side of (38a) exists we can conclude with (66) that

$$\begin{aligned} (\Omega_1)_{[k,l]}(X_{[k,l-1]} I_l) &= (\Omega_1)_{[k,l-1]}(X_{[k,l-1]} I_l), \\ (\Omega_1)_{[k,l]}(I_k X_{[k+1,l]}) &= I_k (\Omega_1)_{[k+1,l]}(X_{[k+1,l]}). \end{aligned} \quad (69)$$

Due to this property one can define Ω_1 as the inductive limit of its restriction

$$\Omega_1 = \lim_{k \rightarrow -\infty} \lim_{l \rightarrow \infty} (\Omega_1)_{[k,l]}. \quad (70)$$

As we shall discuss later the same is also true for the operator Ω_2 .

But before we come to this point let us check whether the limits on the right-hand side of (38a) and (38b) are really well defined.

Proposition 2. *The limits on the right-hand side of equations (38a) and (38b) exist.*

Proof. The existence of the limit in (38b) follows from formula (68), because taking the trace there can result in at most a simple pole $1/(1 - q^\alpha)$. This pole will be cancelled by the factor $(1 - q^{-2\alpha})$ which stands in front of the trace in (68).

In order to prove the existence of the limit in (38a) we use an alternative representation of Ω_1 ,

$$\Omega_1 = - \lim_{\alpha \rightarrow 0} \left[\frac{1}{q^\alpha - q^{-\alpha}} \iint \frac{d\mu_1}{2\pi i} \frac{d\mu_2}{2\pi i} \left(\frac{\zeta_1}{\zeta_2} \right)^\alpha \omega(\mu_2, \mu_1; \alpha) \tilde{\mathbf{X}}(\zeta_1, \zeta_2; \alpha) \right], \quad (71)$$

where⁶

$$\tilde{\mathbf{X}}(\zeta_1, \zeta_2; \alpha) = \text{sing}_{\zeta_1, \zeta_2} [\text{tr}_{a,b} (B_{a,b}(\zeta_1/\zeta_2) \mathbb{T}_b(\zeta_2)^{-1} \mathbb{T}_a(\zeta_1)^{-1}) \mathbf{Q}^-(\zeta_2; \alpha) \mathbf{Q}^+(\zeta_1; \alpha)] \quad (72)$$

with the ‘boundary’ matrix

$$B(\zeta) = \frac{(\zeta - \zeta^{-1})}{2(\zeta q - \zeta^{-1} q^{-1})(\zeta q^{-1} - \zeta^{-1} q)} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \zeta + \zeta^{-1} & -q - q^{-1} & 0 \\ 0 & -q - q^{-1} & \zeta + \zeta^{-1} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (73)$$

and \mathbf{Q}^\pm the same operators as defined in [6],

⁶ Here we take only the spin-0 sector.

$$\mathbf{Q}_{[1,n]}^+(\zeta, \alpha) = \text{tr}_A^+ \left(q^{2\alpha D_A} \mathbb{T}_{A,[1,n]}^+(\zeta)^{-1} \right) (1 - q^{2(\alpha - \mathbb{S})}), \quad (74a)$$

$$\mathbf{Q}_{[1,n]}^-(\zeta, \alpha) = \text{tr}_A^- \left(q^{-2\alpha(D_A+1)} \mathbb{T}_{A,[1,n]}^-(\zeta)^{-1} \right) q^{2\mathbb{S}} (1 - q^{2(\alpha - \mathbb{S})}). \quad (74b)$$

The form (71) of Ω_1 is similar to the form shown in the appendix of [6]. It can be obtained combining the ideas of [4, 6].

The limit in (71) exists, since the integrand is antisymmetric in ζ_1, ζ_2 in the limit $\alpha \rightarrow 0$. This can be seen as follows. First of all $\omega(\mu_2, \mu_1; \alpha)(\zeta_1/\zeta_2)^\alpha$ is symmetric in ζ_1, ζ_2 for $\alpha \rightarrow 0$ (see equation (19)). Next $\text{tr}_{a,b}(B_{a,b}(\zeta_1/\zeta_2)\mathbb{T}_b(\zeta_2)^{-1}\mathbb{T}_a(\zeta_1)^{-1})$ is independent of α and antisymmetric in ζ_1, ζ_2 , since $B(\zeta_1/\zeta_2)$ is antisymmetric in ζ_1, ζ_2 and since $[B(\zeta_1), R(\zeta_2)] = 0$.

It remains to show that $\mathbf{Q}^-(\zeta_2; \alpha)\mathbf{Q}^+(\zeta_1; \alpha)$ is symmetric for $\alpha \rightarrow 0$. This product is meromorphic in α by construction. We show by an explicit calculation in appendix A that it is regular at $\alpha = 0$ and symmetric in ζ_1, ζ_2 in this point. In fact, adopting the notation

$$\mathbf{Q}^\pm(\zeta; 0)(e_{1\sigma_1}^{\varepsilon_1} \cdots e_{n\sigma_n}^{\varepsilon_n}) = \sum_{\sigma'_1, \dots, \sigma'_n; \varepsilon'_1, \dots, \varepsilon'_n} [\mathbf{Q}^\pm(\zeta; 0)]_{\sigma'_1, \dots, \sigma'_n; \varepsilon'_1, \dots, \varepsilon'_n}^{\sigma_1, \dots, \sigma_n; \varepsilon_1, \dots, \varepsilon_n} e_{1\sigma'_1}^{\varepsilon'_1} \cdots e_{n\sigma'_n}^{\varepsilon'_n} \quad (75)$$

for the matrix elements of the operators $\mathbf{Q}^\pm(\zeta; 0)$ with respect to the canonical basis we obtain

$$\begin{aligned} [\mathbf{Q}^\pm(\zeta; 0)]_{\sigma'_1, \dots, \sigma'_n; \varepsilon'_1, \dots, \varepsilon'_n}^{\sigma_1, \dots, \sigma_n; \varepsilon_1, \dots, \varepsilon_n} &= \delta_{\varepsilon_1 + \dots + \varepsilon_n, \sigma_1 + \dots + \sigma_n} \delta_{\varepsilon'_1 + \dots + \varepsilon'_n, \sigma'_1 + \dots + \sigma'_n} \\ &\times \left[\prod_{j=1}^n \frac{\varepsilon_j \varepsilon'_j (\zeta/\xi_j)^{-\frac{1}{2}(\varepsilon_j \varepsilon'_j + \sigma_j \sigma'_j)}}{\zeta/\xi_j - \xi_j/\zeta} \right] q^{\frac{1}{2} \sum_{1 \leq j < k \leq n} ((\varepsilon_j - \varepsilon'_j) \varepsilon'_k - (\sigma_j - \sigma'_j) \sigma'_k)}. \end{aligned} \quad (76)$$

Hence,

$$\mathbf{Q}^-(\zeta_2; 0)\mathbf{Q}^+(\zeta_1; 0) = \mathbf{Q}^+(\zeta_2; 0)\mathbf{Q}^+(\zeta_1; 0) = \mathbf{Q}^+(\zeta_1; 0)\mathbf{Q}^+(\zeta_2; 0) = \mathbf{Q}^-(\zeta_1; 0)\mathbf{Q}^+(\zeta_2; 0), \quad (77)$$

where we used the commutativity $[\mathbf{Q}^+(\zeta_1; \alpha), \mathbf{Q}^+(\zeta_2; \alpha)] = 0$ (see [8]) in the second equation. \square

Following the same lines one can show that the operator Ω_1 is symmetric under the spin reversal transformation,

$$\Omega_1 = \mathbb{J}\Omega_1\mathbb{J}. \quad (78)$$

Moreover, Ω_1 is symmetric under reversal of the direction of the magnetic field

$$\Omega_1 = \Omega_1|_{h \leftrightarrow -h}, \quad (79)$$

since ω is an even function of the magnetic field h . An actual calculation of the right-hand side of equation (38a) or (71) demands to apply l'Hôpital's rule. As a result one gets two terms: one standing with $\omega(\mu_1, \mu_2; 0)$ which is even with respect to the transposition of μ_1 and μ_2 and another one with $\omega'(\mu_1, \mu_2; 0)$ which is odd with respect to $\mu_1 \leftrightarrow \mu_2$. This is the same splitting as discussed in the paper [7]. In section 5, we will consider several examples in order to illustrate this point.

Let us now come to the properties of the operator Ω_2 . We shall consider

$$\mathbf{H}_1(e_{1\sigma_1}^{\varepsilon_1} \cdots e_{n\sigma_n}^{\varepsilon_n}) = \lim_{\alpha \rightarrow 0} \text{res}_{\zeta = \xi_j} \mathbf{H}_{[1,n]}(e_{1\sigma_1}^{\varepsilon_1} \cdots e_{n\sigma_n}^{\varepsilon_n}). \quad (80)$$

In the following we shall need an explicit formula which is also proved in appendix A,

$$\mathbf{H}_1(e_{1\sigma_1}^{\varepsilon_1} \cdots e_{n\sigma_n}^{\varepsilon_n}) = (\mathbf{Q}_{\sigma_1}^{\varepsilon_1} \mathbb{R}_{1;2,\dots,n})(e_{2\sigma_2}^{\varepsilon_2} \cdots e_{n\sigma_n}^{\varepsilon_n}), \quad (81)$$

where the action of the operator $\mathbb{R}_{1;2,\dots,n}$ is defined by

$$\mathbb{R}_{1;2,\dots,n}(X_{[2,n]}) = R_{2,1} \cdots R_{n,1} X_{[2,n]} R_{1,n} \cdots R_{1,2} \quad (82)$$

with the standard R -matrix of the six-vertex model $R_{i,j} = R_{i,j}(\xi_i/\xi_j)$ and where the matrix elements of the operator $\mathbf{Q}_{\sigma_1}^{\varepsilon_1}$ are explicitly given by

$$\begin{aligned} [\mathbf{Q}_{\sigma_1}^{\varepsilon_1}]_{\sigma'_2, \dots, \sigma'_n; \varepsilon_2, \dots, \varepsilon_n}^{\sigma_2, \dots, \sigma_n; \varepsilon_2, \dots, \varepsilon_n} &= \delta_{\varepsilon_1 + \dots + \varepsilon_n, \sigma_1 + \dots + \sigma_n} \delta_{\varepsilon'_2 + \dots + \varepsilon'_n, \sigma'_2 + \dots + \sigma'_n} \\ &\times \frac{\varepsilon_1}{2} \prod_{j=2}^n \frac{\varepsilon_j \varepsilon'_j (\xi_j/\xi_1)^{\frac{\varepsilon_j \varepsilon'_j + \sigma_j \sigma'_j}{2}}}{\xi_j/\xi_1 - \xi_1/\xi_j} q^{\frac{1}{2} \{ (\varepsilon_1 - \sigma_1) \sum_{2 \leq k \leq n} \varepsilon'_k + \sum_{2 \leq j < k \leq n} ((\varepsilon_j - \varepsilon'_j) \varepsilon'_k - (\sigma_j - \sigma'_j) \sigma'_k) \}}. \end{aligned} \quad (83)$$

Note that the limit $\alpha \rightarrow 0$ and the calculation of the residue at $\zeta = \xi_1$ in equation (81) may not be interchanged.

The $\alpha = 0$ limit of the residues at $\zeta = \xi_j$ for $j \geq 2$ can be obtained from formula (81) by applying the exchange relations

$$\check{\mathbb{R}}_{i,i+1} \mathbf{H}_{[1,n]}(\zeta; \alpha)(X_{[1,n]}) = \mathbf{H}_{[1,n]}^{(i,i+1)}(\zeta; \alpha) \check{\mathbb{R}}_{i,i+1}(X_{[1,n]}) \quad (84)$$

with $\mathbf{H}_{[1,n]}^{(i,i+1)} = \mathbf{H}_{[1,n]}|_{\xi_i \leftrightarrow \xi_{i+1}}$ and the action

$$\check{\mathbb{R}}_{i,i+1}(X_{[1,n]}) = \check{R}_{i,i+1} X_{[1,n]} \check{R}_{i,i+1}^{-1} \quad (85)$$

for $1 \leq i, i+1 \leq n$. For example,

$$\mathbf{H}_2(e_1^{\varepsilon_1} \cdots e_n^{\varepsilon_n}) = R_{\varepsilon_2, \varepsilon_1}^{\varepsilon_2, \varepsilon_1}(\xi_2/\xi_1) R_{\sigma_1'', \sigma_2''}^{\sigma_1, \sigma_2}(\xi_1/\xi_2) (\mathbf{Q}_{\sigma_2''}^{\varepsilon_2} \mathbb{R}_{2,3,\dots,n})(e_1^{\varepsilon_1} e_3^{\varepsilon_3} \cdots e_n^{\varepsilon_n}). \quad (86)$$

A most important consequence of the explicit formula (83) is the reduction property.

Proposition 3.

$$\mathbf{H}_1(I_1 e_2^{\varepsilon_2} \cdots e_n^{\varepsilon_n}) = 0, \quad (87a)$$

$$\mathbf{H}_j(I_1 e_2^{\varepsilon_2} \cdots e_n^{\varepsilon_n}) = I_1 \mathbf{H}_j(e_2^{\varepsilon_2} \cdots e_n^{\varepsilon_n}), \quad 2 \leq j \leq n, \quad (87b)$$

$$\mathbf{H}_j(e_1^{\varepsilon_1} \cdots e_{n-1}^{\varepsilon_{n-1}} I_n) = \mathbf{H}_j(e_1^{\varepsilon_1} \cdots e_{n-1}^{\varepsilon_{n-1}}) I_n, \quad 1 \leq j \leq n-1, \quad (87c)$$

$$\mathbf{H}_n(e_1^{\varepsilon_1} \cdots e_{n-1}^{\varepsilon_{n-1}} I_n) = 0. \quad (87d)$$

Proof. The first formula (87a) is rather trivial because from formula (83) it follows that

$$\sum_{\sigma = \pm 1} [\mathbf{Q}_{\sigma}^{\varepsilon}]_{\sigma'_2, \dots, \sigma'_n; \varepsilon_2, \dots, \varepsilon_n}^{\sigma_2, \dots, \sigma_n; \varepsilon_2, \dots, \varepsilon_n} = 0.$$

The second formula (87b) is less trivial. Let us outline the proof for $j = 2$. First we use (86) in order to obtain

$$\mathbf{H}_2(I_1 e_2^{\varepsilon_2} \cdots e_n^{\varepsilon_n}) = R_{\varepsilon_2, \varepsilon_1}^{\varepsilon_2, \varepsilon_1}(\xi_2/\xi_1) R_{\sigma_1'', \sigma_2''}^{\sigma_1, \sigma_2}(\xi_1/\xi_2) (\mathbf{Q}_{\sigma_2''}^{\varepsilon_2} \mathbb{R}_{2,3,\dots,n})(e_1^{\varepsilon_1} e_3^{\varepsilon_3} \cdots e_n^{\varepsilon_n}) \quad (88)$$

and substitute equation (83). The latter should be separated into two parts in such a way that only one of them is touched by two R -matrices on the right-hand side of (88). This part looks like

$$\begin{aligned} &V_{\sigma_1', \sigma_1'', \sigma_2''}^{\varepsilon_1', \varepsilon_1'', \varepsilon_2''}(\xi_1/\xi_2) \\ &:= \frac{1}{2} \varepsilon_1' \varepsilon_1'' \varepsilon_2'' \frac{(\xi_1/\xi_2)^{\frac{1}{2}(\varepsilon_1' \varepsilon_1'' + \sigma_1' \sigma_1'')}}{\xi_1/\xi_2 - \xi_2/\xi_1} \cdot q^{\frac{1}{2}((\varepsilon_2'' - \sigma_2'') \varepsilon_1' - (\sigma_1'' - \sigma_1')(\varepsilon_1' - \sigma_1'))} \cdot q_1^{\frac{1}{2}(\varepsilon_1'' + \varepsilon_2'' - \sigma_1'' - \sigma_2'' - \varepsilon_1' + \sigma_1')}, \end{aligned}$$

where $q_1 = q^{\varepsilon'_3 + \dots + \varepsilon'_n}$ and where the indices $\varepsilon'_3, \dots, \varepsilon'_n$ are considered to be fixed. The following identity can be verified directly, for example, on a computer:

$$V_{\sigma'_1, \sigma'_2}^{\varepsilon'_1, \varepsilon'_2}(\xi_1/\xi_2) R_{\varepsilon'_2, \varepsilon'_1}^{\varepsilon'_2, \varepsilon'_1}(\xi_2/\xi_1) R_{\sigma'_1, \sigma'_2}^{\varepsilon'_1, \varepsilon'_2}(\xi_1/\xi_2) = \frac{1}{2} \delta_{\sigma'_1, \varepsilon'_1} \varepsilon_2 q_1^{\frac{1}{2}(\varepsilon_2 - \sigma_2)}.$$

If we substitute the right-hand side back into (88) and collect all pieces we come to the statement that we wanted to prove, namely,

$$\mathbf{H}_2(I_1 e_{2\sigma_2}^{\varepsilon_2} \dots e_{n\sigma_n}^{\varepsilon_n}) = I_1 \mathbf{H}_2(e_{2\sigma_2}^{\varepsilon_2} \dots e_{n\sigma_n}^{\varepsilon_n}).$$

The other cases when $j > 2$ can be treated in a similar way. Formulae (87c) and (87d) are simple consequences of the inversion of L -operators in the definition (55). \square

Using proposition 3 one immediately comes to the reduction relation for Ω_2 because the restriction of (38b) to the interval $[1, n]$ is

$$(\Omega_2)_{[1, n]} = - \sum_{j=1}^n \varphi(\lambda_j; 0) \mathbf{H}_j. \tag{89}$$

Proposition 4. *Reduction identity for Ω_2 .*

$$(\Omega_2)_{[1, n]}(X_{[1, n-1]} I_n) = (\Omega_2)_{[1, n-1]}(X_{[1, n-1]}) I_n, \tag{90}$$

$$(\Omega_2)_{[1, n]}(I_1 X_{[2, n]}) = I_1 (\Omega_2)_{[2, n]}(X_{[2, n]}).$$

Due to (90) we may define Ω_2 for the infinite chain through an inductive limit as in equation (70).

Another immediate consequence of formula (83) is the spin reversal anti-symmetry. First of all

$$[\mathbf{Q}_{-\sigma_1}^{-\varepsilon_1}]_{-\sigma'_2, \dots, -\sigma'_n; -\varepsilon'_2, \dots, -\varepsilon'_n} = -[\mathbf{Q}_{\sigma_1}^{\varepsilon_1}]_{\sigma'_2, \dots, \sigma'_n; \varepsilon'_2, \dots, \varepsilon'_n}. \tag{91}$$

Then, since the operator $\mathbb{R}_{1; 2, \dots, n}$ is symmetric with respect to the spin reversal transformation,

$$\mathbb{R}_{1; 2, \dots, n} = \mathbb{J}_{[2, n]} \mathbb{R}_{1; 2, \dots, n} \mathbb{J}_{[2, n]}, \tag{92}$$

the operator \mathbf{H}_1 defined by (81) is spin reversal anti-symmetric

$$\mathbf{H}_1 = -\mathbb{J} \mathbf{H}_1 \mathbb{J}. \tag{93}$$

The same is true for the other residues \mathbf{H}_j with $j \geq 2$. Hence, one concludes that

$$\Omega_2 = -\mathbb{J} \Omega_2 \mathbb{J}. \tag{94}$$

Moreover, due to the fact that the function φ given by equation (15) is an odd function of the magnetic field we have

$$\Omega_2 = -\Omega_2|_{h \leftrightarrow -h}. \tag{95}$$

The splitting of the whole operator Ω in equation (37) into two terms Ω_1 and Ω_2 seems rather natural because the two terms are even and odd with respect to the reversal of the spin and the magnetic field, respectively.

5. Examples

In this section, we present explicit formulae for the density matrices for $n = 1, 2$ and for some particular matrix elements and correlation functions for $n = 3$. Since the definition of the operators \mathbf{b} , \mathbf{c} and \mathbf{H} involves the multiplication of $2n$ 2-by-2 matrices and subsequently the calculation of the traces over W^+ or W^- , it is already cumbersome to work out by hand the case $n = 2$. We preferred to use a little computer algebra programme for this task.

5.1. The case $n = 1$

This case is rather simple because $\Omega_1 = 0$ and $\Omega = \Omega_2$. Since $\Omega^2 = \Omega_2^2 = 0$ one should expand the exponent in equation (36) only up to the first order with respect to Ω . A direct calculation shows that the operator \mathbf{H}_1 acts on the basis elements as follows:

$$\mathbf{H}_1(e_{1\pm}) = \pm \frac{1}{2} I_1, \quad \mathbf{H}_1(e_{1\pm\pm}) = 0. \quad (96)$$

Then from (89) one obtains Ω_2 by multiplying the above result by $-\varphi(\lambda_1; 0)$. It is left to substitute it into formula (36) and take the trace $\frac{1}{2} \text{tr}_1$. Finally one obtains the inhomogeneous density matrix:

$$D_1(\lambda_1|T, h; 0) = \frac{1}{2} I_1 - \frac{\varphi(\lambda_1; 0)}{2} \sigma_1^z. \quad (97)$$

In particular, setting $\lambda_1 = 0$ one obtains (see (5) and (8a)) for (twice) the magnetization

$$\langle \sigma_1^z \rangle_{T,h} = \text{tr}_1(D_1(T, h) \sigma_1^z) = -\varphi(0; 0). \quad (98)$$

This result is in full agreement with equation (74) of [22].

5.2. The case $n = 2$

This case is already less trivial. First let us calculate Ω_1 . Using l'Hôpital's rule and the fact that the functions $\omega(\mu_1, \mu_2; 0)$ and $\omega'(\mu_1, \mu_2; 0)$ (recall the definition (20) of ω' !) are even and odd, respectively, with respect to the transposition of μ_1 and μ_2 (see equation (19)) one obtains

$$\Omega_1 = -\omega(\lambda_1, \lambda_2; 0) \Omega_1^+ - \omega'(\lambda_1, \lambda_2; 0) \Omega_1^-, \quad (99)$$

where

$$\begin{aligned} \Omega_1^+ &= \lim_{\alpha \rightarrow 0} (\mathbf{b}_1(\alpha - 1) \mathbf{c}_2(\alpha) (\xi_1/\xi_2)^\alpha + \mathbf{b}_2(\alpha - 1) \mathbf{c}_1(\alpha) (\xi_2/\xi_1)^\alpha), \\ \Omega_1^- &= \lim_{\alpha \rightarrow 0} \alpha (\mathbf{b}_1(\alpha - 1) \mathbf{c}_2(\alpha) (\xi_1/\xi_2)^\alpha - \mathbf{b}_2(\alpha - 1) \mathbf{c}_1(\alpha) (\xi_2/\xi_1)^\alpha), \end{aligned} \quad (100)$$

and

$$\mathbf{b}_j(\alpha) = \text{res}_{\zeta \rightarrow \xi_j} \left(\mathbf{b}(\zeta; \alpha) \frac{d\zeta}{\zeta} \right), \quad \mathbf{c}_j(\alpha) = \text{res}_{\zeta \rightarrow \xi_j} \left(\mathbf{c}(\zeta; \alpha) \frac{d\zeta}{\zeta} \right). \quad (101)$$

The result of applying the operators Ω_1^\pm to the basis of the $S^z = 0$ sector is

$$\begin{aligned} \Omega_1^+(e_{1\epsilon} e_{2\sigma}) &= -\frac{\epsilon\sigma}{4} \text{cth}(\eta) I_1 I_2, & \Omega_1^+(e_{1-\epsilon} e_{2-\epsilon}) &= \frac{1}{4} \frac{\text{ch}(\lambda_1 - \lambda_2)}{\text{sh}(\eta)} I_1 I_2, \\ \Omega_1^-(e_{1\epsilon} e_{2\sigma}) &= -\frac{\epsilon\sigma}{4\eta} \text{cth}(\lambda_1 - \lambda_2) I_1 I_2, & \Omega_1^-(e_{1-\epsilon} e_{2-\epsilon}) &= \frac{1}{4\eta} \frac{\text{ch}(\eta)}{\text{sh}(\lambda_1 - \lambda_2)} I_1 I_2. \end{aligned} \quad (102)$$

It is clear that

$$(\Omega_1^\pm)^2 = \Omega_1^+ \Omega_1^- = \Omega_1^- \Omega_1^+ = 0 \quad (103)$$

which implies

$$\Omega_1^2 = 0. \quad (104)$$

Also the symmetry with respect to spin reversal is obvious in the explicit formulae (102).

Let us proceed with the anti-symmetric part. To obtain \mathbf{H}_j for $j = 1, 2$ one can either take the corresponding residues in formula (68) or one can use formulae (81) for $j = 1$ and (86) for $j = 2$. The result is

$$\begin{aligned}\mathbf{H}_1(e_{1_\varepsilon^\varepsilon}e_{2_\sigma^\sigma}) &= \frac{\varepsilon}{2}(f_1^{\varepsilon\sigma}(\xi_1, \xi_2)e_{1_\varepsilon^\varepsilon}e_{2_\varepsilon^\varepsilon} + f_1^{-\varepsilon\sigma}(\xi_1, \xi_2)e_{1_{-\varepsilon}^-}e_{2_{-\varepsilon}^-} + f_2^{\varepsilon\sigma}(\xi_1, \xi_2)e_{1_\varepsilon^\varepsilon}e_{2_{-\varepsilon}^-} \\ &\quad + f_2^{-\varepsilon\sigma}(\xi_1, \xi_2)e_{1_{-\varepsilon}^-}e_{2_\varepsilon^\varepsilon} - \sigma g_1(\xi_1, \xi_2)(e_{1_+^-}e_{2_+^-} - e_{1_+^+}e_{2_+^+})), \\ \mathbf{H}_1(e_{1_{-\varepsilon}^-}e_{2_{-\varepsilon}^-}) &= \frac{1}{2}(q^{-1}f_3^\varepsilon(\xi_1, \xi_2)e_{1_\varepsilon^\varepsilon}e_{2_\varepsilon^\varepsilon} + qf_3^{-\varepsilon}(\xi_1, \xi_2)e_{1_{-\varepsilon}^-}e_{2_{-\varepsilon}^-} + \varepsilon q^{-1}g_2^+(\xi_1, \xi_2)e_{1_\varepsilon^\varepsilon}e_{2_{-\varepsilon}^-} \\ &\quad - \varepsilon qg_2^-(\xi_1, \xi_2)e_{1_{-\varepsilon}^-}e_{2_\varepsilon^\varepsilon} + g_3(\xi_1, \xi_2)(e_{1_+^-}e_{2_+^-} - e_{1_+^+}e_{2_+^+}))\end{aligned}\quad (105)$$

and

$$\begin{aligned}\mathbf{H}_2(e_{1_\varepsilon^\varepsilon}e_{2_\sigma^\sigma}) &= \frac{\sigma}{2}(f_1^-(\xi_1, \xi_2)e_{1_\varepsilon^\varepsilon}I_2 + f_1^+(\xi_1, \xi_2)e_{1_{-\varepsilon}^-}I_2), \\ \mathbf{H}_2(e_{1_{-\varepsilon}^-}e_{2_{-\varepsilon}^-}) &= -\frac{\varepsilon}{2}(q^{-1}f_3^+(\xi_1, \xi_2)e_{1_\varepsilon^\varepsilon}I_2 + qf_3^-(\xi_1, \xi_2)e_{1_{-\varepsilon}^-}I_2),\end{aligned}\quad (106)$$

where

$$\begin{aligned}f_1^+(\xi_1, \xi_2) &:= \frac{1}{1 - \xi_1^2/\xi_2^2}, \\ f_2^+(\xi_1, \xi_2) &:= \frac{(q - q^{-1})^2 + (1 - \xi_1^2/\xi_2^2)^2}{(1 - \xi_1^2/\xi_2^2)(q\xi_1/\xi_2 - q^{-1}\xi_2/\xi_1)(q\xi_2/\xi_1 - q^{-1}\xi_1/\xi_2)}, \\ f_3^+(\xi_1, \xi_2) &:= \frac{1}{\xi_1/\xi_2 - \xi_2/\xi_1}, \quad \text{and} \quad f_i^-(\xi_1, \xi_2) := f_i^+(\xi_2, \xi_1).\end{aligned}\quad (107)$$

$$\begin{aligned}g_1(\xi_1, \xi_2) &:= \frac{(\xi_1/\xi_2 + \xi_2/\xi_1)(q - q^{-1})}{(q\xi_1/\xi_2 - q^{-1}\xi_2/\xi_1)(q\xi_2/\xi_1 - q^{-1}\xi_1/\xi_2)}, \\ g_2^\pm(\xi_1, \xi_2) &:= \frac{(q - q^{-1})^2 + q^{\pm 2}(\xi_1/\xi_2 - \xi_2/\xi_1)^2}{(\xi_1/\xi_2 - \xi_2/\xi_1)(q\xi_1/\xi_2 - q^{-1}\xi_2/\xi_1)(q\xi_2/\xi_1 - q^{-1}\xi_1/\xi_2)}, \\ g_3(\xi_1, \xi_2) &:= \frac{q^2 - q^{-2}}{(q\xi_1/\xi_2 - q^{-1}\xi_2/\xi_1)(q\xi_2/\xi_1 - q^{-1}\xi_1/\xi_2)}.\end{aligned}\quad (108)$$

The anti-symmetry of the operators \mathbf{H}_1 and \mathbf{H}_2 with respect to the spin reversal transformation is evident in the above formulae.

Also one can directly verify that

$$\mathbf{H}_1^2 = \mathbf{H}_2^2 = \mathbf{H}_1\mathbf{H}_2 + \mathbf{H}_2\mathbf{H}_1 = 0 \quad (109)$$

and

$$\mathbf{H}_j\Omega_1 + \Omega_1\mathbf{H}_j = 0, \quad j = 1, 2. \quad (110)$$

This means that the operator Ω_2 which is

$$\Omega_2 = -\varphi(\lambda_1; 0)\mathbf{H}_1 - \varphi(\lambda_2; 0)\mathbf{H}_2 \quad (111)$$

satisfies

$$\Omega_2^2 = \Omega_1\Omega_2 + \Omega_2\Omega_1 = 0. \quad (112)$$

From this follows that

$$\Omega^2 = 0 \quad (113)$$

and the expansion of the exponent in formula (36) extends only up to the first order in powers of Ω .

Therefore in order to compute the elements of the density matrix we need to calculate the traces

$$D_{2\sigma_1, \sigma_2}^{\varepsilon_1, \varepsilon_2}(\lambda_1, \lambda_2 | T, h; 0) = \frac{1}{4} \text{tr}_1 \text{tr}_2 [(\text{id} + \Omega_1 + \Omega_2)(e_{1\varepsilon_1}^{\sigma_1} e_{2\varepsilon_2}^{\sigma_2})]. \quad (114)$$

For this purpose we have to use formulae (99), (102) and (111), (105), (106). The result decomposes as follows:

$$D_2(\lambda_1, \lambda_2 | T, h; 0) = D_2^{\text{even}}(\lambda_1, \lambda_2) + D_2^{\text{odd}}(\lambda_1, \lambda_2), \quad (115)$$

where D_2^{even} and D_2^{odd} are 4×4 matrices,

$$\begin{aligned} D_2^{\text{even}}(\lambda_1, \lambda_2) &= \frac{1}{4} I \otimes I + \frac{1}{4} \left[\text{cth}(\eta) \omega(\lambda_1, \lambda_2; 0) + \frac{\text{cth}(\lambda_1 - \lambda_2)}{\eta} \omega'(\lambda_1, \lambda_2; 0) \right] \sigma^z \otimes \sigma^z \\ &\quad - \frac{1}{4} \left[\frac{\text{ch}(\lambda_1 - \lambda_2)}{\text{sh}(\eta)} \omega(\lambda_1, \lambda_2; 0) + \frac{\text{ch}(\eta)}{\eta \text{sh}(\lambda_1 - \lambda_2)} \omega'(\lambda_1, \lambda_2; 0) \right] (\sigma^+ \otimes \sigma^- + \sigma^- \otimes \sigma^+) \end{aligned} \quad (116)$$

and

$$\begin{aligned} D_2^{\text{odd}}(\lambda_1, \lambda_2) &= -\frac{\varphi(\lambda_1; 0)}{4} \sigma^z \otimes I - \frac{\varphi(\lambda_2; 0)}{4} I \otimes \sigma^z \\ &\quad - \frac{\text{sh}(\eta)(\varphi(\lambda_1; 0) - \varphi(\lambda_2; 0))}{4 \text{sh}(\lambda_1 - \lambda_2)} (\sigma^+ \otimes \sigma^- - \sigma^- \otimes \sigma^+). \end{aligned} \quad (117)$$

The homogeneous limit $\lambda_1, \lambda_2 \rightarrow 0$ can be readily taken. We obtain the density matrix for $n = 2$,

$$\begin{aligned} D_2(T, h) &= \frac{1}{4} \left[I \otimes I - \varphi(\sigma^z \otimes I + I \otimes \sigma^z) - \text{sh}(\eta) \varphi_x (\sigma^+ \otimes \sigma^- - \sigma^- \otimes \sigma^+) \right. \\ &\quad \left. + \left(\text{cth}(\eta) \omega + \frac{\omega'_x}{\eta} \right) \sigma^z \otimes \sigma^z - \left(\frac{\omega}{\text{sh}(\eta)} + \frac{\text{ch}(\eta) \omega'_x}{\eta} \right) (\sigma^+ \otimes \sigma^- + \sigma^- \otimes \sigma^+) \right], \end{aligned} \quad (118)$$

where we introduced the shorthand notation

$$\begin{aligned} \varphi &= \varphi(0; 0), & \varphi_x &= \partial_\lambda \varphi(\lambda; 0)|_{\lambda=0}, \\ \omega &= \omega(0, 0; 0), & \omega'_x &= \partial_{\lambda_1} \omega'(\lambda_1, \lambda_2; 0)|_{\lambda_1, \lambda_2=0}. \end{aligned} \quad (119)$$

The density matrix (118) can now be used to obtain any two-site correlation function, e.g.,

$$\langle \sigma_1^z \sigma_2^z \rangle_{T, h} = \text{tr}_{12} (D_2(T, h) \sigma_1^z \sigma_2^z) = \text{cth}(\eta) \omega + \frac{\omega'_x}{\eta}, \quad (120a)$$

$$\langle \sigma_1^x \sigma_2^x \rangle_{T, h} = \text{tr}_{12} (D_2(T, h) \sigma_1^x \sigma_2^x) = -\frac{\omega}{2 \text{sh}(\eta)} - \frac{\text{ch}(\eta) \omega'_x}{2\eta}. \quad (120b)$$

The density matrix $D_2(T, h)$ simplifies in various limits. For vanishing magnetic field $\varphi = \varphi_x = 0$, and the second and third terms in (118) vanish. Performing the $T \rightarrow 0$ limit we can replace ω with the explicit integral shown in the introduction of [6]. It is a useful and simple exercise to confirm (118) in the free fermion limit $\Delta = 0$ for h, T finite (compare [23]).

5.3. The case $n = 3$

The explicit forms of Ω_j or \mathbf{H}_j are already quite involved for $n = 3$. We shall not present the exhausting list of matrix elements, but rather restrict ourselves to some examples of physical interest.

We introduce shorthand notations

$$\begin{aligned} \mathfrak{d}_1^{\varepsilon_1, \varepsilon_2} &= f_1^{\varepsilon_1}(\xi_2, \xi_3) f_1^{\varepsilon_2}(\xi_3, \xi_1), & \mathfrak{d}_2^{\varepsilon_1, \varepsilon_2} &= f_1^{\varepsilon_1}(\xi_1, \xi_2) f_1^{\varepsilon_2}(\xi_3, \xi_1), \\ \mathfrak{d}_3^{\varepsilon_1, \varepsilon_2} &= f_1^{\varepsilon_1}(\xi_1, \xi_2) f_1^{\varepsilon_2}(\xi_2, \xi_3), & \mathfrak{t}^{\varepsilon_1, \varepsilon_2, \varepsilon_3} &= f_1^{\varepsilon_1}(\xi_1, \xi_2) f_1^{\varepsilon_2}(\xi_2, \xi_3) f_1^{\varepsilon_3}(\xi_3, \xi_1). \end{aligned} \quad (121)$$

Using these symbols, the longitudinal correlation is represented rather compactly. In the inhomogeneous case we find

$$\begin{aligned} \text{tr}_{123} (D_3(\lambda_1, \lambda_2, \lambda_3 | T, h; 0) \sigma_1^z \sigma_3^z) &= \text{th}(\eta) (\mathfrak{d}_1^{++} + \mathfrak{d}_1^{--}) \omega(\lambda_1, \lambda_2; 0) + \text{th}(\eta) (\mathfrak{d}_2^{++} + \mathfrak{d}_2^{--}) \omega(\lambda_2, \lambda_3; 0) \\ &+ (2\text{cth}(2\eta) (\mathfrak{d}_3^{++} + \mathfrak{d}_3^{--}) + \text{cth}(\eta) (\mathfrak{d}_3^{+-} + \mathfrak{d}_3^{-+})) \omega(\lambda_3, \lambda_1; 0) \\ &- \frac{4\text{sh}^2(\eta)}{\eta} \mathfrak{t}^{+++} (\omega'(\lambda_1, \lambda_2; 0) + \omega'(\lambda_2, \lambda_3; 0)) \\ &- \frac{1}{\eta} (4\text{ch}^2(\eta) \mathfrak{t}^{+++} - (\mathfrak{t}^{+-} + \mathfrak{t}^{-+} + \mathfrak{t}^{--})) \\ &+ \mathfrak{t}^{+-} + \mathfrak{t}^{-+} + \mathfrak{t}^{--} \omega'(\lambda_3, \lambda_1; 0). \end{aligned} \quad (122)$$

Taking the homogeneous limit we arrive at

$$\langle \sigma_1^z \sigma_3^z \rangle_{T, h} = 2\text{cth}(2\eta) \omega + \frac{1}{4} \text{th}(\eta) \omega_{xx} - \frac{1}{2} \text{th}(\eta) \omega_{xy} + \frac{\omega'_x}{\eta} - \frac{\text{sh}^2(\eta)}{4\eta} \omega'_{xy}. \quad (123)$$

By x and y we denote the derivatives with respect to first and second argument taken at zero. The same limit for the transverse correlation reads as follows:

$$\begin{aligned} \langle \sigma_1^+ \sigma_3^- + \sigma_1^- \sigma_3^+ \rangle_{T, h} &= -\frac{1}{\text{sh}(2\eta)} \omega + \frac{\text{ch}(2\eta) \text{th}(\eta)}{4} \omega_{xy} - \frac{\text{ch}(2\eta) \text{th}(\eta)}{8} \omega_{xx} - \frac{\text{ch}(2\eta)}{2\eta} \omega'_x + \frac{\text{sh}^2(\eta)}{8\eta} \omega'_{xy}. \end{aligned} \quad (124)$$

The rational limit in the last two equations is not easy. Using the high-temperature expansion we checked to $\mathcal{O}(1/T)$ that it coincides with our previous result [1] for the XXX chain.

As a last example we show the emptiness formation probability in the inhomogeneous case:

$$\begin{aligned} D_{+++}(\lambda_1, \lambda_2, \lambda_3 | T, h; 0) &= \frac{1}{8} + \frac{1}{8} (-\varphi(\lambda_3; 0) + C_1(\xi_1, \xi_2, \xi_3) \omega(\lambda_1, \lambda_2; 0) \\ &+ C_2(\xi_1, \xi_2, \xi_3) \omega'(\lambda_1, \lambda_2; 0) + C_3(\xi_1, \xi_2, \xi_3) \omega(\lambda_1, \lambda_2; 0) \varphi(\lambda_3; 0) \\ &+ C_4(\xi_1, \xi_2, \xi_3) \omega'(\lambda_1, \lambda_2; 0) \varphi(\lambda_3; 0) + \text{cyclic permutations}). \end{aligned} \quad (125)$$

Here the coefficients are given as follows:

$$\begin{aligned} C_1(\xi_1, \xi_2, \xi_3) &= (2\text{cth}(2\eta) (\mathfrak{d}_1^{++} + \mathfrak{d}_1^{--}) + \text{cth}(\eta) (\mathfrak{d}_1^{+-} + \mathfrak{d}_1^{-+})), \\ C_2(\xi_1, \xi_2, \xi_3) &= \frac{1}{\eta} (-2\text{ch}(2\eta) \mathfrak{t}^{+++} - (\mathfrak{t}^{+-} + \mathfrak{t}^{-+} + \mathfrak{t}^{--}) + \mathfrak{t}^{--} + \mathfrak{t}^{-+} + \mathfrak{t}^{--}), \\ C_3(\xi_1, \xi_2, \xi_3) &= \text{cth}(\eta) (2(\mathfrak{d}_1^{++} + \mathfrak{d}_1^{--}) - (\mathfrak{d}_1^{+-} + \mathfrak{d}_1^{-+})), \\ C_4(\xi_1, \xi_2, \xi_3) &= \frac{1}{\eta} (-4\text{ch}^2(\eta) \mathfrak{t}^{+++} + \mathfrak{t}^{+-} + \mathfrak{t}^{-+} + \mathfrak{t}^{--} - (\mathfrak{t}^{--} + \mathfrak{t}^{-+} + \mathfrak{t}^{--})). \end{aligned} \quad (126)$$

The homogeneous limit is left as an exercise to the reader.

6. Conclusions

In an attempt to generalize the recent results [6, 8] on the factorization of the ground-state correlation functions of the XXZ chain to include finite temperatures and a finite longitudinal magnetic field we have constructed a conjectural exponential formula (37), (38) for the density matrix. The main steps in our work were the construction of the operator \mathbf{H} , equation (55), which takes care of the modification of the algebraic part of the exponential formula in the presence of a magnetic field, and of the functions φ and ω , equations (15), (17), which allowed us to give a description of the physical part in close analogy to [6, 8]. In the limit $T, h \rightarrow 0$ our conjecture reduces to the result of [6, 8], even for finite α . It also trivializes in the expected way as $T \rightarrow \infty$. We tested our conjecture against the multiple integral formula (9) by direct comparison for $n = 2$ (see appendix B) and by comparison of the high-temperature expansion data for $n = 3$ and $n = 4$. Judging from our experience with the isotropic case [17] we find it likely that very similar formulae also hold in the finite length case and that the only modifications necessary to cover this case are a restriction of Ω to the finite length L of the chain and a change of the auxiliary function from (10) to (14).

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Appendix A. Proof of equations (76) and (83)

Here we outline the proof of equations (76) and (83). Our starting point is equation (74a). Since we work in the sector $S^z = 0$, we have to set $\mathbb{S} = 0$. Then

$$[\mathbf{Q}^+(\zeta; \alpha)]_{\sigma'_1, \dots, \sigma'_n; \varepsilon'_1, \dots, \varepsilon'_n}^{\sigma_1, \dots, \sigma_n; \varepsilon_1, \dots, \varepsilon_n} = (1 - q^{2\alpha}) \times \text{tr}_A^+ \left((L_A^+(\zeta/\xi_1)^{-1})_{\sigma'_1}^{\sigma_1} \dots (L_A^+(\zeta/\xi_n)^{-1})_{\sigma'_n}^{\sigma_n} (L_A^+(\zeta/\xi_n))_{\varepsilon_n}^{\varepsilon'_n} \dots (L_A^+(\zeta/\xi_1))_{\varepsilon_1}^{\varepsilon'_1} q^{2\alpha D_A} \right), \quad (\text{A.1})$$

where $(L_A^+(\zeta))_{\varepsilon}^{\varepsilon'}$ are the matrix elements of the L -operator (51a),

$$(L_A^+(\zeta))_{\varepsilon}^{\varepsilon'} = i\zeta^{-\frac{1}{2}} q^{-\frac{1}{4}} \begin{pmatrix} q^{D_A} & -\zeta a_A^* q^{-D_A} \\ -\zeta a_A q^{D_A} & q^{-D_A} - \zeta^2 q^{D_A+2} \end{pmatrix}_{\varepsilon, \varepsilon'} \quad (\text{A.2})$$

and

$$(L_A^+(\zeta)^{-1})_{\varepsilon}^{\varepsilon'} = \frac{i\zeta^{-\frac{1}{2}} q^{\frac{1}{4}}}{\zeta - \zeta^{-1}} \begin{pmatrix} q^{-D_A} - \zeta^2 q^{D_A} & \zeta q^{-D_A} a_A^* \\ \zeta q^{D_A} a_A & q^{D_A} \end{pmatrix}_{\varepsilon, \varepsilon'}. \quad (\text{A.3})$$

The main observation is that for the computation of the limit $\alpha \rightarrow 0$ of equation (A.1) it is enough to substitute there L_A^+ and $(L_A^+)^{-1}$ by \tilde{L}_A^+ and $(\tilde{L}_A^+)^{-1}$ with⁷

$$(\tilde{L}_A^+(\zeta))_{\varepsilon}^{\varepsilon'} = i\zeta^{-\frac{1}{2}} q^{-\frac{1}{4}} \begin{pmatrix} q^{D_A} & -\zeta a_A^* q^{-D_A} \\ -\zeta a_A q^{D_A} & q^{-D_A} \end{pmatrix}_{\varepsilon, \varepsilon'} = i\zeta^{-\frac{1}{2}} q^{-\frac{1}{4}} \varepsilon \varepsilon' \zeta^{\frac{1-\varepsilon\varepsilon'}{2}} a_A^{-\frac{\varepsilon-\varepsilon'}{2}} q^{\varepsilon' D_A} \quad (\text{A.4})$$

⁷ Strictly speaking the operators \tilde{L}_A^+ and $(\tilde{L}_A^+)^{-1}$ are not inverse to each other any longer.

and

$$(\tilde{L}_A^+(\zeta)^{-1})_{\varepsilon'}^{\varepsilon'} = \frac{i\zeta^{-\frac{1}{2}}q^{\frac{1}{4}}}{\zeta - \zeta^{-1}} \begin{pmatrix} q^{-D_A} & \zeta q^{-D_A} a_A^* \\ \zeta q^{D_A} a_A & q^{D_A} \end{pmatrix}_{\varepsilon, \varepsilon'} = \frac{i\zeta^{-\frac{1}{2}}q^{\frac{1}{4}}}{\zeta - \zeta^{-1}} \zeta^{\frac{1-\varepsilon\varepsilon'}{2}} q^{-\varepsilon D_A} a_A^{-\frac{\varepsilon-\varepsilon'}{2}}, \quad (\text{A.5})$$

where we set

$$a_A^+ = a_A, \quad a_A^- = a_A^*. \quad (\text{A.6})$$

In this notation the algebra (48) looks very simple

$$a_A^\varepsilon q^{\varepsilon' D_A} = q^{\varepsilon\varepsilon'} q^{\varepsilon' D_A} a_A^\varepsilon. \quad (\text{A.7})$$

The reason is as follows. Let us first formally substitute \tilde{L}_A^+ and $(\tilde{L}_A^+)^{-1}$ for L_A^+ and $(L_A^+)^{-1}$ into the right-hand side of equation (A.1),

$$(1 - q^{2\alpha}) \prod_{j=1}^n \frac{\varepsilon_j \varepsilon'_j (\zeta/\xi_j)^{-\frac{1}{2}(\varepsilon_j \varepsilon'_j + \sigma_j \sigma'_j)}}{\zeta/\xi_j - \xi_j/\zeta} \text{tr}_A^+ (q^{-\sigma'_1 D_A} a_A^{-\frac{1}{2}(\sigma'_1 - \sigma_1)} \dots q^{-\sigma'_n D_A} a_A^{-\frac{1}{2}(\sigma'_n - \sigma_n)} \\ \times a_A^{-\frac{1}{2}(\varepsilon_n - \varepsilon'_n)} q^{\varepsilon'_n D_A} \dots a_A^{-\frac{1}{2}(\varepsilon_1 - \varepsilon'_1)} q^{\varepsilon'_1 D_A} q^{2\alpha D_A}). \quad (\text{A.8})$$

We do not write the δ 's like on the right-hand side of (76) which reflect the fact that we are in the spin-0 sector. Let us just imply that they are there.

Let us formally ignore all a_A^\pm inside the trace here. Then the total degree of q^{D_A} is zero because $\sum_j \varepsilon'_j = \sum_j \sigma'_j$, and only $q^{2\alpha D_A}$ is left, which produces a term $1/(1 - q^{2\alpha})$ after taking the trace over the oscillator space A . Since the differences between L_A^+ and \tilde{L}_A^+ and between $(L_A^+)^{-1}$ and $(\tilde{L}_A^+)^{-1}$ contain only positive powers of q^{D_A} , the insertion of such terms does not change that most singular term $1/(1 - q^{2\alpha})$ when $\alpha \rightarrow 0$. Therefore we can ignore those differences when calculating the limit $\alpha \rightarrow 0$.

One more observation is about the contribution coming from the terms containing a_A^\pm . Suppose we had just

$$\text{tr}_A^+ (a_A^{\varepsilon_1} \dots a_A^{\varepsilon_{2n}} q^{2\alpha D_A})$$

with $\varepsilon_1 + \dots + \varepsilon_{2n} = 0$. Then, using the algebra (48) we would conclude that again the most singular term would be $1/(1 - q^{2\alpha})$ as a result of taking the trace. It means that if one succeeds in collecting all a_A^\pm then one can replace them by 1 without any change in the most singular term. The first conclusion obtained from the above is that the limit $\alpha \rightarrow 0$ of the expression (A.8) gives us the limit $\alpha \rightarrow 0$ of equation (A.1). Second, in order to calculate it we have to collect all a_A^\pm inside the trace (A.8) using the algebra (A.7) in one place, say in the place of the symbol \times in (A.8). If we do this and afterwards ignore the product of all a_A^\pm following the above arguments, then we can easily take the limit $\alpha \rightarrow 0$ and come to formula (76). Similar arguments may be applied when treating the $\alpha \rightarrow 0$ limit of formula (74b).

Now we outline the derivation of formula (83). When calculating the residue at ξ_1 which is implied in equation (81) one obtains

$$[\mathbf{Q}_{\sigma_1}^{\varepsilon_1}]_{\sigma_2', \dots, \sigma_n'; \varepsilon_2', \dots, \varepsilon_n'}^{\sigma_2, \dots, \sigma_n; \varepsilon_2, \dots, \varepsilon_n} = \lim_{\alpha \rightarrow 0} \text{res}_{\zeta=\xi_1} \text{tr}_A^+ ((L_A^+(\zeta/\xi_1)^{-1})_{\sigma}^{\sigma_1} (L_A^+(\zeta/\xi_2)^{-1})_{\sigma_2'}^{\sigma_2} \dots (L_A^+(\zeta/\xi_n)^{-1})_{\sigma_n'}^{\sigma_n} \\ \times (L_A^+(\zeta/\xi_n))_{\varepsilon_n}^{\varepsilon_n'} \dots (L_A^+(\zeta/\xi_2))_{\varepsilon_2}^{\varepsilon_2'} (L_A^+(\zeta/\xi_1))_{\varepsilon_1}^{\varepsilon_1'} q^{2\alpha D_A}), \quad (\text{A.9})$$

where summation over σ is implied. The pole at $\zeta = \xi_1$ originates from the L -operators with argument ζ/ξ_1 . We use the cyclicity of the trace and directly verify that

$$\text{res}_{\zeta=\xi_1} (L_A^+(\zeta/\xi_1))_{\varepsilon_1}^{\sigma} q^{2\alpha D_A} (L_A^+(\zeta/\xi_1)^{-1})_{\sigma}^{\sigma_1} = -\frac{q^\alpha - q^{-\alpha}}{2} \left[\begin{pmatrix} 1 \\ -a_A \end{pmatrix} a_A^* (q^{-\alpha} a_A, q^\alpha) \right]_{\varepsilon_1, \sigma_1} q^{2\alpha D_A}. \quad (\text{A.10})$$

Implying that we need to calculate the limit $\alpha \rightarrow 0$ in the end we may set

$$(1 - q^\alpha) \left[\begin{pmatrix} 1 \\ -a_A \end{pmatrix} (1, a_A^*) \right]_{\varepsilon_1, \sigma_1} q^{2\alpha D_A} = (1 - q^\alpha) \varepsilon_1 a^{-\frac{1}{2}(\varepsilon_1 - \sigma_1)} q^{2\alpha D_A} \quad (\text{A.11})$$

on the right-hand side of (A.10). Thus, we come to the conclusion that the right-hand side of (A.9) is equal to

$$\lim_{\alpha \rightarrow 0} \left[(1 - q^\alpha) \text{tr}_A^+ \left((L_A^+(\xi_1/\xi_2)^{-1})_{\sigma'_2}^{\sigma_2} \cdots (L_A^+(\xi_1/\xi_n)^{-1})_{\sigma'_n}^{\sigma_n} \right. \right. \\ \left. \left. \times (L_A^+(\xi_1/\xi_n))_{\varepsilon_n}^{\varepsilon'_n} \cdots (L_A^+(\xi_1/\xi_2))_{\varepsilon_2}^{\varepsilon'_2} \varepsilon_1 a^{-\frac{1}{2}(\varepsilon_1 - \sigma_1)} q^{2\alpha D_A} \right) \right]. \quad (\text{A.12})$$

Finally we can apply to equation (A.12) the same trick as described above in order to get formula (83).

Appendix B. Factorization of the double integral

In this appendix, we show that our conjectured formula for the density matrix for $n = 2$, equations (115)–(117), coincides with the double integral, equation (9) for $n = 2$. The density matrix for $n = 2$ has six non-vanishing elements. In this appendix, we will denote it by D rather than by D_2 and suppress the temperature, magnetic field and α dependence of the matrix elements for short. Using the Yang–Baxter algebra and reduction we find four independent relations between the six non-vanishing matrix elements of D ,

$$\begin{aligned} D_{+-}^+(\lambda_1, \lambda_2) &= D_+^+(\lambda_1) - D_{++}^{++}(\lambda_1, \lambda_2), & D_{-+}^-(\lambda_1, \lambda_2) &= D_+^+(\lambda_2) - D_{++}^{++}(\lambda_1, \lambda_2), \\ D_{--}^-(\lambda_1, \lambda_2) &= D_{++}^{++}(\lambda_1, \lambda_2) - D_+^+(\lambda_1) - D_+^+(\lambda_2) + 1, \\ D_{+-}^-(\lambda_1, \lambda_2) - D_{-+}^+(\lambda_1, \lambda_2) &= \frac{\text{sh}(\eta)(D_+^+(\lambda_1) - D_+^+(\lambda_2))}{\text{sh}(\lambda_1 - \lambda_2)}. \end{aligned} \quad (\text{B.1})$$

Inserting these relations into $D(\lambda_1, \lambda_2|T, h; 0)$ we obtain

$$\begin{aligned} D(\lambda_1, \lambda_2|T, h; 0) &= \frac{1}{4}I \otimes I + \frac{1}{4}(2D_+^+(\lambda_1) - 1)\sigma^z \otimes I + \frac{1}{4}(2D_+^+(\lambda_2) - 1)I \otimes \sigma^z \\ &+ \frac{1}{4}(4D_{++}^{++}(\lambda_1, \lambda_2) - 2D_+^+(\lambda_1) - 2D_+^+(\lambda_2) + 1)\sigma^z \otimes \sigma^z \\ &+ \frac{1}{2}(D_{+-}^-(\lambda_1, \lambda_2) + D_{-+}^+(\lambda_1, \lambda_2))(\sigma^+ \otimes \sigma^- + \sigma^- \otimes \sigma^+) \\ &+ \frac{\text{sh}(\eta)}{2\text{sh}(\lambda_1 - \lambda_2)}(D_+^+(\lambda_1) - D_+^+(\lambda_2))(\sigma^+ \otimes \sigma^- - \sigma^- \otimes \sigma^+), \end{aligned} \quad (\text{B.2})$$

and we are left with the problem of expressing the one-point function $D_+^+(\lambda)$ and the two-point functions $D_{++}^{++}(\lambda_1, \lambda_2)$ and $D_{+-}^-(\lambda_1, \lambda_2) + D_{-+}^+(\lambda_1, \lambda_2)$ in terms of φ and ω .

Comparing (9) for $n = 1$ with the definition (15) of our function φ we find the relation

$$2D_+^+(\lambda) = 1 - \varphi(\lambda; 0) \quad (\text{B.3})$$

for the one-point function.

In order to simplify our task for the two-point functions we introduce the quantum group invariant combination [4]:

$$D_q(\lambda_1, \lambda_2) = e^{\lambda_1 - \lambda_2} D_{-+}^{+-}(\lambda_1, \lambda_2) + e^{\lambda_2 - \lambda_1} D_{+-}^{-+}(\lambda_1, \lambda_2) - e^{-\eta} D_{-+}^{+-}(\lambda_1, \lambda_2) - e^{\eta} D_{+-}^{-+}(\lambda_1, \lambda_2). \quad (\text{B.4})$$

Using again (B.1) we obtain the relation

$$\begin{aligned} \text{ch}(\lambda_1 - \lambda_2)(D_{-+}^{+-}(\lambda_1, \lambda_2) + D_{+-}^{-+}(\lambda_1, \lambda_2)) \\ = D_q(\lambda_1, \lambda_2) + \text{ch}(\eta)(D_+^+(\lambda_1) + D_+^+(\lambda_2) - 2D_{++}^{++}(\lambda_1, \lambda_2)). \end{aligned} \quad (\text{B.5})$$

Hence, in order to determine the density matrix for $n = 2$, it suffices to calculate $D_q(\lambda_1, \lambda_2)$ and $D_{++}^+(\lambda_1, \lambda_2)$ from the double integrals.

Let us start with the simpler case $D_q(\lambda_1, \lambda_2)$. Inserting (9) into the definition (B.4) we find

$$D_q(\lambda_1, \lambda_2) = \int_C \frac{d\omega_1}{2\pi i(1 + \mathfrak{a}(\omega_1))} \int_C \frac{d\omega_2}{2\pi i(1 + \bar{\mathfrak{a}}(\omega_2))} \det[-G(\omega_j, \lambda_k; 0)] r(\omega_1, \omega_2), \quad (\text{B.6})$$

where

$$r(\omega_1, \omega_2) = -\frac{e^{\lambda_1 + \lambda_2} \text{sh}(\lambda_1 - \lambda_2 + \eta) \text{sh}(\lambda_1 - \lambda_2 - \eta)}{e^{\omega_1 + \omega_2} \text{sh}(\lambda_1 - \lambda_2) \text{sh}(\omega_1 - \omega_2 - \eta)}. \quad (\text{B.7})$$

Using the simple relation

$$\frac{1}{1 + \mathfrak{a}(\omega)} + \frac{1}{1 + \bar{\mathfrak{a}}(\omega)} = 1 \quad (\text{B.8})$$

we can rewrite (B.6) as

$$\begin{aligned} D_q(\lambda_1, \lambda_2) &= \int_C \frac{d\omega}{2\pi i(1 + \mathfrak{a}(\omega))} (r(\omega, \lambda_1)G(\omega, \lambda_2; 0) - r(\omega, \lambda_2)G(\omega, \lambda_1; 0)) \\ &\quad - \frac{1}{2} \int_C \frac{d\omega_1}{2\pi i(1 + \mathfrak{a}(\omega_1))} \int_C \frac{d\omega_2}{2\pi i(1 + \mathfrak{a}(\omega_2))} \\ &\quad \times \det[-G(\omega_j, \lambda_k; 0)] (r(\omega_1, \omega_2) - r(\omega_2, \omega_1)). \end{aligned} \quad (\text{B.9})$$

The first term on the right-hand side is already a single integral. For the second term we observe that

$$-\frac{1}{2}(r(\omega_1, \omega_2) - r(\omega_2, \omega_1)) = \frac{\text{ch}(\eta)(e^{-2\omega_1} - e^{-2\omega_2}) \text{sh}(\lambda_1 - \lambda_2 + \eta) \text{sh}(\lambda_1 - \lambda_2 - \eta)}{(e^{-2\lambda_1} - e^{-2\lambda_2}) \text{sh}(\omega_1 - \omega_2 + \eta) \text{sh}(\omega_1 - \omega_2 - \eta)}. \quad (\text{B.10})$$

The ω -dependent terms in the denominator are proportional to the kernel in the integral equation (11) for $\alpha = 0$, and the numerator is a sum of a function of ω_1 and a function of ω_2 . Hence, the double integral can be reduced to single integrals by means of the integral equation (11). Collecting the resulting terms and inserting the definition (16) of our function ψ we arrive at

$$D_q(\lambda_1, \lambda_2) = \frac{\text{sh}(\lambda_1 - \lambda_2 + \eta) \text{sh}(\lambda_1 - \lambda_2 - \eta)}{2\text{sh}(\eta)} \psi(\lambda_1, \lambda_2; 0). \quad (\text{B.11})$$

Let us proceed with the calculation of $D_{++}^+(\lambda_1, \lambda_2)$ which according to (9) is equal to

$$\begin{aligned} D_{++}^+(\lambda_1, \lambda_2) &= \lim_{\alpha \rightarrow 0} \int_C \frac{d\omega_1 e^{-\alpha\eta}}{2\pi i(1 + \mathfrak{a}(\omega_1))} \int_C \frac{d\omega_2 e^{-\alpha\eta}}{2\pi i(1 + \mathfrak{a}(\omega_2))} \\ &\quad \times \det[-G(\omega_j, \lambda_k; \alpha)] \underbrace{\frac{\text{sh}(\omega_1 - \lambda_1 - \eta) \text{sh}(\omega_2 - \lambda_2)}{\text{sh}(\lambda_2 - \lambda_1) \text{sh}(\omega_1 - \omega_2 - \eta)}}_{=s(\omega_1, \omega_2)}. \end{aligned} \quad (\text{B.12})$$

Because of the antisymmetry of the determinant we may replace $s(\omega_1, \omega_2)$ with

$$\begin{aligned} &\frac{1}{2}(s(\omega_1, \omega_2) - s(\omega_2, \omega_1)) \\ &= \frac{\text{ch}(\eta)(\text{sh}(2\omega_2 - \lambda_1 - \lambda_2 - \eta) - \text{sh}(2\omega_1 - \lambda_1 - \lambda_2 - \eta)) + \text{ch}(\lambda_1 - \lambda_2) \text{sh}(2(\omega_1 - \omega_2))}{4\text{sh}(\lambda_1 - \lambda_2) \text{sh}(\omega_1 - \omega_2 + \eta) \text{sh}(\omega_1 - \omega_2 - \eta)}. \end{aligned}$$

Then

$$D_{++}^+(\lambda_1, \lambda_2) = J_1(\lambda_1, \lambda_2) + \lim_{\alpha \rightarrow 0} J_2(\lambda_1, \lambda_2; \alpha), \quad (\text{B.13})$$

where

$$J_1(\lambda_1, \lambda_2) = \left[\prod_{j=1}^2 \int_C \frac{d\omega_j}{2\pi i(1 + \mathfrak{a}(\omega_j))} \right] \frac{\det[G(\omega_j, \lambda_k; 0)] \operatorname{ch}(\eta) \operatorname{sh}(2\omega_2 - \lambda_1 - \lambda_2 - \eta)}{2\operatorname{sh}(\omega_1 - \omega_2 + \eta) \operatorname{sh}(\omega_1 - \omega_2 - \eta) \operatorname{sh}(\lambda_1 - \lambda_2)},$$

$$J_2(\lambda_1, \lambda_2; \alpha) = \left[\prod_{j=1}^2 \int_C \frac{d\omega_j e^{-\alpha\eta}}{2\pi i(1 + \mathfrak{a}(\omega_j))} \right] \frac{\det[G(\omega_j, \lambda_k; \alpha)] \operatorname{cth}(\lambda_1 - \lambda_2) \operatorname{sh}(2(\omega_1 - \omega_2))}{4\operatorname{sh}(\omega_1 - \omega_2 + \eta) \operatorname{sh}(\omega_1 - \omega_2 - \eta)}.$$

Here $J_1(\lambda_1, \lambda_2)$ is of a form which allows us to carry out one integration by means of (11) (for $\alpha = 0$). The result is

$$J_1(\lambda_1, \lambda_2) = \frac{1}{2} - \frac{1}{4}(\varphi(\lambda_1; 0) + \varphi(\lambda_2; 0)) - \frac{1}{4} \operatorname{cth}(\eta) \psi(\lambda_1, \lambda_2; 0) + \frac{1}{2} \operatorname{cth}(\lambda_1 - \lambda_2) \sum_{P \in \mathfrak{S}^2} \operatorname{sign}(P) \int_C \frac{d\omega G(\omega, \lambda_{P1}; 0) \operatorname{cth}(\omega - \lambda_{P2} - \eta)}{2\pi i(1 + \mathfrak{a}(\omega))}. \quad (\text{B.14})$$

For the calculation of $J_2(\lambda_1, \lambda_2; \alpha)$ we express the hyperbolic functions in the integrand in terms of the kernel (12) occurring in the integral equation (11) for G ,

$$\frac{\operatorname{sh}(2(\omega_1 - \omega_2))}{\operatorname{sh}(\omega_1 - \omega_2 + \eta) \operatorname{sh}(\omega_1 - \omega_2 - \eta)} = \frac{K(\omega_1 - \omega_2; \alpha) - K(\omega_2 - \omega_1; \alpha)}{2\operatorname{sh}(\alpha\eta)}. \quad (\text{B.15})$$

Then the integral over ω_2 can be performed by means of the integral equation (11) for finite α , and we obtain

$$J_2(\lambda_1, \lambda_2; \alpha) = -\frac{1}{4} e^{-2\alpha\eta} \operatorname{cth}(\lambda_1 - \lambda_2) \frac{\psi(\lambda_1, \lambda_2; \alpha) - \psi(\lambda_2, \lambda_1; \alpha)}{2\operatorname{sh}(\alpha\eta)} - \frac{1}{2} e^{-2\alpha\eta} \operatorname{cth}(\lambda_1 - \lambda_2) \sum_{P \in \mathfrak{S}^2} \operatorname{sign}(P) \int_C \frac{d\omega G(\omega, \lambda_{P1}; \alpha) \operatorname{cth}(\omega - \lambda_{P2} - \eta)}{2\pi i(1 + \mathfrak{a}(\omega))}. \quad (\text{B.16})$$

From the definition (16) of ψ and from the integral equation (11) for G we infer the symmetry property $\psi(\lambda_2, \lambda_1; \alpha) = \psi(\lambda_1, \lambda_2; -\alpha)$ which can be used to carry out the limit $\alpha \rightarrow 0$ for J_2 . Using it and inserting the $\alpha \rightarrow 0$ limit of (B.16) and (B.14) into (B.13) we arrive at

$$D_{++}^{++}(\lambda_1, \lambda_2) = \frac{1}{2} - \frac{1}{4}(\varphi(\lambda_1; 0) + \varphi(\lambda_2; 0)) - \frac{\operatorname{cth}(\eta)}{4} \psi(\lambda_1, \lambda_2; 0) - \frac{\operatorname{cth}(\lambda_1 - \lambda_2)}{4\eta} \psi'(\lambda_1, \lambda_2; 0), \quad (\text{B.17})$$

where the prime denotes the derivative with respect to α . Inserting now (B.5), (B.11) and (B.17) into (B.2) and taking into account the definitions (17) and (20) of ω and ω' the reader will readily reproduce the density matrix (115)–(117) for $n = 2$.

Appendix C. The high-temperature expansions

We comment on the application of high-temperature expansions (HTE) to the multiple integral formula, which provide important data for the construction of the conjectures in this report. This may also be a basis for the numerical evaluation of correlations as demonstrated in [42, 41].

As is usual, we assume an expansion of quantities in regular powers of $\frac{1}{T}$. We then typically face the problem of solving a linear integral equation for a unknown function $f(\lambda)$,

$$f(\lambda) = f_0(\lambda) + \nu \int_C \frac{d\omega}{2\pi i} K(\lambda - \omega; \alpha) f(\omega) := f_0(\lambda) + \nu K * f(\lambda), \quad (\text{C.1})$$

where ν stands for some constant. The driving term $f_0(\lambda)$ is a known function which has at most simple poles at $\lambda = \mu_i$ and a pole of certain order at $\lambda = 0$ inside \mathcal{C} . Equation (C.1) can be solved in an iterative manner,

$$f(\lambda) = f_0(\lambda) + \nu K * f_0(\lambda) + \nu^2 K * (K * f_0)(\lambda) + \dots \quad (\text{C.2})$$

The crucial observation is that $K * f_0(\lambda)$ has poles at $\lambda = \pm\eta, \mu_i \pm \eta$ and that these poles are outside of contour \mathcal{C} . Thus, only the first two terms in (C.2) do not vanish and $f(\lambda) = f_0(\lambda) + \nu K * f_0(\lambda)$ solves equation (C.1).

This mechanism makes it possible to evaluate each order in the HTE in an analytic and exact manner. Of course, the evaluation of residues becomes more and more involved with increasing order of $\frac{1}{T}$. Computer programs like Mathematica, however, can efficiently cope with such a task and we obtain sufficiently many data for our purpose.

Here we present some examples which one can compute by hand. We consider the nonlinear integral equation (10) under the assumption

$$\mathfrak{a}(\lambda) = 1 + \frac{\mathfrak{a}^{(1)}(\lambda)}{T} + \frac{\mathfrak{a}^{(2)}(\lambda)}{T^2} + \dots$$

Then comparing $O(\frac{1}{T})$ terms, one obtains the equation,

$$\mathfrak{a}^{(1)}(\lambda) = a_0(\lambda) - \frac{1}{2} \int_{\mathcal{C}} \frac{d\omega}{2\pi i} K(\lambda - \omega; 0) \mathfrak{a}^{(1)}(\omega), \quad a_0(\lambda) = -h - \frac{2J \operatorname{sh}^2(\eta)}{\operatorname{sh}(\lambda) \operatorname{sh}(\lambda + \eta)}.$$

We apply the above strategy and find the first thermal correction to $\mathfrak{a}(\lambda)$ as

$$\mathfrak{a}^{(1)}(\lambda) = -h + \frac{2J \operatorname{sh}^3(\eta) \operatorname{ch}(\lambda)}{\operatorname{sh}(\lambda) \operatorname{sh}(\lambda - \eta) \operatorname{sh}(\lambda + \eta)}.$$

Similarly the first correction to $\bar{\mathfrak{a}}(\lambda)$ is found to be $\bar{\mathfrak{a}}^{(1)}(\lambda) = -\mathfrak{a}^{(1)}(\lambda)$.

Equation (11) can be solved similarly. Let $G(\lambda, \mu; \alpha) = G^{(0)}(\lambda, \mu; \alpha) + G^{(1)}(\lambda, \mu; \alpha)/T + \dots$. Then the following explicit forms are obtained:

$$\begin{aligned} G^{(0)}(\lambda, \mu; \alpha) &= -\operatorname{coth}(\lambda - \mu) + e^{\alpha\eta} \frac{\operatorname{coth}(\lambda - \mu - \eta)}{2} + e^{-\alpha\eta} \frac{\operatorname{coth}(\lambda - \mu + \eta)}{2}, \\ G^{(1)}(\lambda, \mu; \alpha) &= -h \frac{K(\lambda - \mu; \alpha)}{4} + \frac{J \operatorname{sh}^3(\eta) \operatorname{ch}(\mu) K(\lambda - \mu; \alpha)}{2 \operatorname{sh}(\mu) \operatorname{sh}(\mu - \eta) \operatorname{sh}(\mu + \eta)} \\ &\quad + \frac{J \operatorname{sh} \eta K(\lambda; \alpha) G^{(0)}(0, \mu; \alpha)}{2}. \end{aligned}$$

All elements of the density matrix can now be evaluated up to $O(T^{-1})$. A simple example is the emptiness formation probability for $n = 2$,

$$\begin{aligned} D_{++}^{++}(\lambda_1, \lambda_2 | T, h; 0) &= \frac{1}{4} + \frac{\mathfrak{a}^{(1)}(\lambda_1) + \mathfrak{a}^{(1)}(\lambda_2)}{8T} - \frac{J \operatorname{sh} \eta G^{(0)}(0, \lambda_2; 0)}{4T} \frac{\operatorname{sh} \lambda_1 \operatorname{sh}(\lambda_2 - \lambda_1 + \eta)}{\operatorname{sh}(\lambda_2 - \lambda_1) \operatorname{sh}(\lambda_1 - \eta)} \\ &\quad - \frac{J \operatorname{sh} \eta G^{(0)}(0, \lambda_1; 0)}{4T} \frac{\operatorname{sh} \lambda_2 \operatorname{sh}(\lambda_1 - \lambda_2 + \eta)}{\operatorname{sh}(\lambda_1 - \lambda_2) \operatorname{sh}(\lambda_2 - \eta)} + O(T^{-2}). \end{aligned}$$

The other basic functions are also readily evaluated:

$$\begin{aligned} \varphi(\mu; \alpha) &= -\frac{h}{2T} + \frac{J \operatorname{sh} \eta}{2T} ((1 - e^{-\alpha\eta}) \operatorname{coth}(\mu - \eta) + (1 - e^{\alpha\eta}) \operatorname{coth}(\mu + \eta)) + O(T^{-2}), \\ \psi(\mu_1, \mu_2; \alpha) &= -\frac{1}{2} K(\mu_1 - \mu_2; -\alpha) + \frac{(\mathfrak{a}^{(1)}(\mu_2) - \mathfrak{a}^{(1)}(\mu_1)) G^{(0)}(\mu_2, \mu_1; \alpha)}{2T} \\ &\quad - \frac{J \operatorname{sh} \eta}{T} G^{(0)}(0, \mu_1; \alpha) G^{(0)}(\mu_2, 0; \alpha) + O(T^{-2}). \end{aligned}$$

One can then check the validity of our conjecture by comparing the multiple integral formula for the density matrix and the exponential formula after substitution of the basic functions by their HTE data up to $O(T^{-1})$. The higher order terms can, in principle, be checked in the same manner.

Before closing the paper, we sketch briefly how we used the HTE data to arrive at our conjecture. Each density matrix element consists of two parts; D^{even} , the even part with respect to the magnetic field, and D^{odd} , the odd part. The factorization for $n = 2$ can be done fully in an analytic manner, as demonstrated in appendix B. This result and the previous results of the XXX case motivate us to assume that the even part shares the same algebraic part with the ground-state case. Then it is not difficult to identify two basic functions, $\phi(\lambda_1, \lambda_2)$, $\tilde{\phi}(\lambda_1, \lambda_2)$. We can actually represent them by the single function $\psi(\lambda_1, \lambda_2; \alpha)$ such that $\phi(\lambda_1, \lambda_2) = \frac{\text{sh}\eta}{2} \psi(\lambda_1, \lambda_2; 0)$, $\tilde{\phi}(\lambda_1, \lambda_2) = -\frac{\text{sh}\eta}{2\eta} \frac{\partial}{\partial \alpha} \psi(\lambda_1, \lambda_2; \alpha)|_{\alpha=0}$. This is one of the advantages in using the disorder parameter α .

We then consider the odd part of $n = 3$. The most interesting sector is $D_3^{\text{odd}\varepsilon_1, \varepsilon_2, \varepsilon_3}_{\sigma_1, \sigma_2, \sigma_3}(\lambda_1, \lambda_2, \lambda_3)$ with $\sum_i \varepsilon_i = \sum_i \sigma_i = 1$ to which nine elements belong. With use of the Yang–Baxter relation and the intrinsic symmetry of the density matrix, one can represent all the element by only one element. We choose $D_3^{\text{odd}++-}$ for this, with permutations of the arguments $(\lambda_1, \lambda_2, \lambda_3)$. The resulting 6 objects are found to satisfy linear algebraic relations, and the consideration of the kernel space implies the representation

$$D_3^{\text{odd}++-}(\xi_1, \xi_2, \xi_3) = \frac{s_1(\xi_1, \xi_2, \xi_3)}{\xi_2} + \frac{s_2(\xi_1, \xi_2, \xi_3)}{\xi_1 \xi_3},$$

where $\xi_i = e^{\lambda_i}$, and s_1, s_2 denote certain symmetric functions of ξ_j .

We then assume that s_1, s_2 are given by sums of products of rational functions of x_i and the basic functions φ, ϕ and $\tilde{\phi}$, e.g.,

$$s_1(\xi_1, \xi_2, \xi_3) = V_0(\xi_1, \xi_2|\xi_3)\varphi(\xi_3; 0) + V_1(\xi_1, \xi_2|\xi_3)\varphi(\xi_3; 0)\phi(\xi_1, \xi_2) \\ + \tilde{V}_1(\xi_1, \xi_2|\xi_3)\varphi(\xi_3; 0)\tilde{\phi}(\xi_1, \xi_2) + \text{cyclic permutations.}$$

$V_j(\xi_1, \xi_2|\xi_3)$ is symmetric in ξ_1, ξ_2 ($j = 0, 1$) while $\tilde{V}_1(\xi_1, \xi_2|\xi_3)$ is anti-symmetric.

Furthermore, we restrict the possible forms of these coefficients according to our previous experience such that

$$V_0(\xi_1, \xi_2|\xi_3) = \frac{p_0(\xi_1, \xi_2|\xi_3)}{(\xi_1^2 - \xi_3^2)(\xi_2^2 - \xi_3^2)}, \quad V_1(\xi_1, \xi_2|\xi_3) = \frac{p_1(\xi_1, \xi_2|\xi_3)}{(\xi_1^2 - \xi_3^2)(\xi_2^2 - \xi_3^2)}, \\ \tilde{V}_1(\xi_1, \xi_2|\xi_3) = \frac{\tilde{p}_1(\xi_1, \xi_2|\xi_3)}{(\xi_1^2 - \xi_3^2)(\xi_2^2 - \xi_3^2)(\xi_1^2 - \xi_2^2)}.$$

Now p_j and \tilde{p}_1 are polynomials in ξ_i and p_j (\tilde{p}_1) is symmetric (anti-symmetric) in ξ_1, ξ_2 . We then assume polynomials of certain orders with desired symmetry for them and fix the unknown coefficients so as to match the HTE data. All these parameters are fortunately fixed by the data up to $O(T^{-3})$. At the final stage, several hundreds of terms are cancelled just by fixing one parameter, which looks rather convincing. We then check that the choice of parameters actually recovers the $O(T^{-4})$ terms in the HTE. After this procedure, we arrive at expressions for the density matrix elements now written in terms of rational functions and basic functions. We then try to fit them into the exponential formula. This requires the new operator \mathbf{H} in the main body. Once it is identified, it is easy to write down the conjecture for $n = 4$. Then again we test the validity against the HTE data for the multiple integral formulae of the density matrix.

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