Density matrices for finite segments of Heisenberg chains of arbitrary length

Density matrices for finite segments of Heisenberg chains of arbitrary length

Jens Damerau, Frank Göhmann, Nils P Hasenclever
and Andreas Klümper

Fachbereich C—Physik, Bergische Universität Wuppertal, 42097 Wuppertal, Germany

E-mail: damerau@physik.uni-wuppertal.de, goehmann@physik.uni-wuppertal.de, hasenclever@physik.uni-wuppertal.de and kluemper@physik.uni-wuppertal.de

Abstract

We derive a multiple integral representing the ground-state density matrix of a segment of length m of the *XXZ* spin chain on L lattice sites, which depends on L only parametrically. This allows us to treat chains of arbitrary finite length. Specializing to the isotropic limit of the *XXX* chain we show for small m that the multiple integrals factorize. We conjecture that this property holds for arbitrary m and suggest an exponential formula for the density matrix which involves only a double Cauchy type integral in the exponent. We demonstrate the efficiency of our formula by computing the next-to-nearest neighbour zz-correlation function for chain lengths ranging from two to macroscopic numbers.

PACS numbers: 05.30.−d, 75.10.Pq

1. Introduction

Formally, integrable systems at finite temperature have much in common with finite-length systems. In the former case, the free energy in the thermodynamic limit can be expressed as the logarithm of the dominant eigenvalue of a quantum transfer matrix [23, 24], whereas in the latter case the logarithmic derivative of the largest eigenvalue of the usual row-to-row transfer matrix [1] determines the ground-state energy of the system of length L. In both cases the technique of nonlinear integral equations [20, 21] can be applied to express the transfer matrix eigenvalue as an integral over appropriately defined auxiliary functions. The integrals can be evaluated numerically yielding high precision data for thermodynamic properties at arbitrary temperatures, or for the ground-state energy at arbitrary lengths, respectively.

Here we show for the *XXZ* spin-1/2 chain that this formal similarity persists for a multiple integral representation of the density matrix of a chain segment which was first derived for the ground state of the infinitely long chain [15, 16, 19] and later generalized to finite temperature [10, 12]. We also show examples which suggest that the factorization of the multiple integrals,

that was proven for the ground state of the infinite chain at vanishing magnetic field [3, 6, 7] and recently observed at finite temperature and nonzero magnetic field [2], might also generally hold for the ground state of a finite chain.

2. The *XXZ* chain and its integrable structure

The *XXZ* chain is an anisotropic generalization of the Heisenberg spin chain. If the value of all local spins is $1/2$ the model is integrable, and its Hamiltonian can be expressed through the local action of the Pauli matrices σ^x, σ^y, σ^z on L sites of a chain,

$$H = J \sum_{j=1}^{L} \left(\sigma_{j-1}^x \sigma_j^x + \sigma_{j-1}^y \sigma_j^y + \Delta \left(\sigma_{j-1}^z \sigma_j^z - 1 \right) \right). \tag{1}$$

This Hamiltonian depends on two real parameters, the exchange coupling J and an anisotropy parameter Δ. We shall consider the critical antiferromagnetic regime $J > 0$, $-1 < \Delta \leqslant 1$. Setting $\Theta = \mathrm{diag}(\mathrm{e}^{\mathrm{i}\Phi}, \mathrm{e}^{-\mathrm{i}\Phi})$, $\Phi \in [0, 2\pi]$, we fix the boundary conditions requiring that

$$\begin{pmatrix} e_{0\,1}^1 & e_{0\,2}^1 \\ e_{0\,1}^2 & e_{0\,2}^2 \end{pmatrix} = \Theta \begin{pmatrix} e_{L\,1}^1 & e_{L\,2}^1 \\ e_{L\,1}^2 & e_{L\,2}^2 \end{pmatrix} \Theta^{-1}, \tag{2}$$

where the e_β^α, $\alpha, \beta = 1, 2$, denote the gl(2) standard basis $\left(\sigma^x = e_2^1 + e_1^2, \sigma^y = \mathrm{i}\left(e_2^1 - e_1^2\right), \sigma^z = e_1^1 - e_2^2 \right)$. We call Φ the twist angle. $\Phi = 0$ corresponds to the familiar periodic boundary conditions.

All results in this paper rely heavily on the fact that H can be derived from the well-known trigonometric R-matrix

$$R(\lambda) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & b(\lambda) & c(\lambda) & 0 \\ 0 & c(\lambda) & b(\lambda) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{3}$$

$$b(\lambda) = \frac{\mathrm{sh}(\lambda)}{\mathrm{sh}(\lambda + \eta)}, \qquad c(\lambda) = \frac{\mathrm{sh}(\eta)}{\mathrm{sh}(\lambda + \eta)}, \tag{4}$$

of the six-vertex model [1]. Associating a 2×2 L-matrix with elements

$$L_{j\,\beta}^{\,\alpha}(\lambda) = R_{\beta\delta}^{\alpha\gamma}(\lambda) e_{j\,\gamma}^{\,\delta} \tag{5}$$

with every lattice site we can define the monodromy matrix of the *XXZ* chain,

$$T(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix} = \Theta L_L(\lambda) \cdots L_1(\lambda). \tag{6}$$

It provides, by construction, a representation of the Yang–Baxter algebra,

$$\check{R}(\lambda - \mu)(T(\lambda) \otimes T(\mu)) = (T(\mu) \otimes T(\lambda))\check{R}(\lambda - \mu), \tag{7}$$

where $\check{R} = PR$ if P is the transposition of the two factors in $\mathbb{C}^2 \otimes \mathbb{C}^2$. We define the twisted transfer matrix $t(\lambda) = \mathrm{tr}\, T(\lambda)$. Then, due to (7), the function $\ln(t^{-1}(0)t(\lambda))$ generates a sequence of commuting local operators. The first one is proportional to the Hamiltonian (1),

$$H = 2J\mathrm{sh}(\eta)\partial_\lambda \ln(t^{-1}(0)t(\lambda))|_{\lambda=0}, \tag{8}$$

with twisted boundary conditions (2) if we identify $\Delta = \mathrm{ch}(\eta)$. The critical regime corresponds to purely imaginary $\eta = \mathrm{i}\gamma$, $\gamma \in [0, \pi)$. Because of (8) we may solve the eigenvalue problem of the transfer matrix rather than dealing directly with the Hamiltonian.

3. The Bethe ansatz solution for the ground state

The twisted transfer matrix $t(\lambda)$ can be diagonalized by means of the algebraic Bethe ansatz. Since this technique has been explained elsewhere (see e.g. [22]), we may be content here with a mere description of the result. Eigenstates $|\{\lambda\}\rangle$ of $t(\lambda)$ are generated by the multiple action of the operators $B(\lambda)$, equation (6), on the ferromagnetic state $|0\rangle = \left(\begin{smallmatrix}1\\0\end{smallmatrix}\right)^{\otimes L}$,

$$|\{\lambda\}\rangle = B\left(\lambda_1 - \frac{\eta}{2}\right) \cdots B\left(\lambda_N - \frac{\eta}{2}\right)|0\rangle. \tag{9}$$

Here the set of so-called Bethe roots $\{\lambda\} = \{\lambda_j\}_{j=1}^N$ is not arbitrary, but must be determined from the Bethe ansatz equations:

$$1 + \frac{e^{-2i\Phi}sh^L\left(\lambda_j - \frac{\eta}{2}\right)}{sh^L\left(\lambda_j + \frac{\eta}{2}\right)} \prod_{k=1}^N \frac{sh(\lambda_j - \lambda_k + \eta)}{sh(\lambda_j - \lambda_k - \eta)} = 0, \qquad j = 1, \ldots, N. \tag{10}$$

The transfer matrix eigenvalues corresponding to the eigenstates (9) are given by

$$\Lambda(\lambda) = e^{i\Phi} \prod_{j=1}^N \frac{sh\left(\lambda - \lambda_j - \frac{\eta}{2}\right)}{sh\left(\lambda - \lambda_j + \frac{\eta}{2}\right)} + \frac{e^{-i\Phi}sh^L(\lambda)}{sh^L(\lambda + \eta)} \prod_{j=1}^N \frac{sh\left(\lambda - \lambda_j + \frac{3\eta}{2}\right)}{sh\left(\lambda - \lambda_j + \frac{\eta}{2}\right)}. \tag{11}$$

In the following we shall concentrate on the ground-state properties of the *XXZ* chain. This brings about severe simplifications. We will be dealing with a single rather special solution of the Bethe ansatz equations, and we do not have to touch the delicate question under which circumstances the set of states (9) is complete. Let us fix an even length L of the chain. Then the ground state of the Hamiltonian (1) is the transfer matrix eigenstate (9) with $\{\lambda_j\}_{j=1}^{L/2}$ the unique real solution of (10) for $N = L/2$. The real and mutually distinct Bethe roots in this solution uniquely determine a meromorphic auxiliary function

$$\mathfrak{a}(\lambda) = \frac{e^{-2i\Phi}sh^L\left(\lambda - \frac{\eta}{2}\right)}{sh^L\left(\lambda + \frac{\eta}{2}\right)} \prod_{k=1}^{L/2} \frac{sh(\lambda - \lambda_k + \eta)}{sh(\lambda - \lambda_k - \eta)} \tag{12}$$

in the complex plane. In terms of this function the ground-state eigenvalue $\Lambda_0(\lambda)$ becomes

$$\Lambda_0(\lambda) = \left(1 + \mathfrak{a}\left(\lambda + \frac{\eta}{2}\right)\right) e^{i\Phi} \prod_{j=1}^{L/2} \frac{sh\left(\lambda - \lambda_j - \frac{\eta}{2}\right)}{sh\left(\lambda - \lambda_j + \frac{\eta}{2}\right)}. \tag{13}$$

It follows from the Bethe ansatz equations that $\Lambda_0(\lambda)$ is regular at the points $\lambda_j - \frac{\eta}{2}$, $j = 1, \ldots, L/2$. Extensive numerical studies moreover support the conjecture that $\Lambda_0(\lambda)$ is nonzero inside a strip $-|\eta| \leqslant \text{Im}\,\lambda \leqslant 0$. Our following treatment of the ground state of the finite-size system is based on this conjecture. It has strong immediate consequences. It implies that the function $1 + \mathfrak{a}(\lambda)$ is analytic inside the strip $-\frac{|\eta|}{2} < \text{Im}\,\lambda \leqslant \frac{|\eta|}{2}$ and that its only zeros in this strip are the Bethe roots. This together with the obvious analytic and asymptotic properties of $\mathfrak{a}(\lambda)$ is enough to set up a set of functional equations for the second logarithmic derivatives of $\mathfrak{a}(\lambda)$ and $1 + \mathfrak{a}(\lambda)$ which together with their known asymptotics determine $\mathfrak{a}(\lambda)$ uniquely [21]. Once the functional equations are formulated it is easy to transform them into nonlinear integral equations. This procedure is, however, non-unique. We usually work with two alternative forms of the nonlinear integral equations. One (we call it the '$\mathfrak{a}$-form') is convenient for theoretical purposes. We shall use it in order to write the density matrix as a multiple integral. The other form (we call it the '$\mathfrak{b}\bar{\mathfrak{b}}$-form') is useful for numerical calculations. The $\mathfrak{b}\bar{\mathfrak{b}}$-form was first derived in [21]. We show it later when we demonstrate the numerical efficiency of our formulae. Here is the $\mathfrak{a}$-form of the nonlinear integral equation:

$$\ln \mathfrak{a}(\lambda) = -2i\Phi + L\eta + L \ln\left(\frac{sh\left(\lambda - \frac{\eta}{2}\right)}{sh\left(\lambda + \frac{\eta}{2}\right)}\right) - \int_{\mathcal{C}} \frac{d\omega}{2\pi} K_\eta(\lambda - \omega) \ln(1 + \mathfrak{a}(\omega)). \tag{14}$$
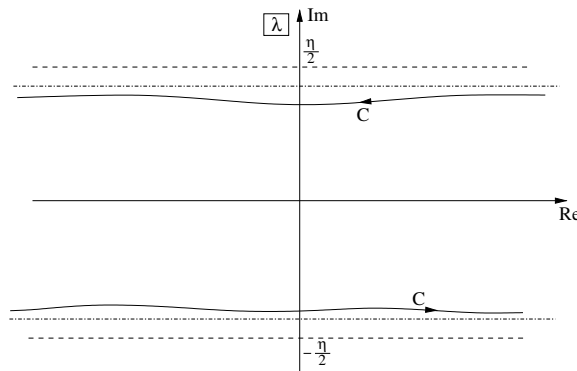
Figure 1. The canonical contour $\mathcal{C}$ surrounds the real axis in counterclockwise manner inside the strip $-\frac{|\eta|}{2} < \operatorname{Im}\lambda < \frac{|\eta|}{2}$.

The integration contour $\mathcal{C}$ is shown in figure 1. It surrounds the real axis in counterclockwise manner. The kernel $K_\eta(\lambda)$ is defined as

$$K_\eta(\lambda) = \frac{\operatorname{sh}(2\eta)}{\operatorname{ish}(\lambda - \eta)\operatorname{sh}(\lambda + \eta)}. \tag{15}$$

We claim that inside the strip $-\frac{|\eta|}{2} \leqslant \operatorname{Im}\lambda \leqslant \frac{|\eta|}{2}$ the function $\mathfrak{a}(\lambda)$ as defined in (14) is the same as the function $\mathfrak{a}(\lambda)$ as defined in (12) and (10) with $N = L/2$. The ground-state eigenvalue $\Lambda_0(\lambda)$ can also be expressed as an integral over $\mathfrak{a}(\lambda)$:

$$\ln \Lambda_0(\lambda) = \mathrm{i}\Phi + \frac{L(\mathrm{i}\pi - \eta)}{2} + \int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi} K_{\frac{\eta}{2}}(\lambda - \omega) \ln(1 + \mathfrak{a}(\omega)). \tag{16}$$

This determines the ground-state energy and the eigenvalues of the higher conserved quantities as a function of L.

Another implication of the fact that the function $1 + \mathfrak{a}(\lambda)$ is analytic inside the strip $-\frac{|\eta|}{2} < \operatorname{Im}\lambda \leqslant \frac{|\eta|}{2}$ and that its only zeros in this strip are the Bethe roots is the formula

$$\int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{f(\omega)}{1 + \mathfrak{a}(\omega)} = \sum_{j=1}^{L/2} \frac{f(\lambda_j)}{\mathfrak{a}'(\lambda_j)} \tag{17}$$

which holds for any function $f(\lambda)$ analytic in the strip. This formula, when read from right to left, enables us to rewrite sums over the ground-state Bethe roots as integrals over the 'canonical contour' $\mathcal{C}$. It is one of the key tools in the derivation of the integral representation for the density matrix shown in the next section.

4. The density matrix as a multiple integral

The density matrix is a means to describe a sub-system as part of a larger system in thermodynamic equilibrium in terms of the degrees of freedom of the sub-system. Typically the system is divided into two parts, interpreted as sub-system and environment. Then one is usually interested in the limit when the sub-system is kept fixed and the size of the environment goes to infinity. Here we shall keep both parts finite and study the influence of the size of the environment on the sub-system which will be a segment consisting of the first $m < L$ lattice sites of the *XXZ* chain. The environment will consist of the remaining sites.

Let

$$\rho_L = \frac{e^{-\frac{H}{T}}}{\operatorname{tr} e^{-\frac{H}{T}}} \tag{18}$$

be the statistical operator for the chain at temperature T. Then the density matrix of the sub-system consisting of the first m lattice sites is defined as

$$D_L(T) = \operatorname{tr}_{m+1\cdots L} \rho_L. \tag{19}$$

By construction, the thermal average of every operator A acting non-trivially only on sites 1 to m can now be written as

$$\langle A \rangle_T = \operatorname{tr}_{1\cdots L} A \rho_L = \operatorname{tr}_{1\cdots m} A_{1\cdots m} \operatorname{tr}_{m+1\cdots L} \rho_L = \operatorname{tr}_{1\cdots m} A_{1\cdots m} D_L(T), \tag{20}$$

where $A_{1\cdots m}$ is the restriction of A to a chain consisting of sites 1 to m. In particular, every two-point function of local operators in the segment 1 to m of the *XXZ* chain can be brought into the above form. If we follow the common convention and use the same symbols for the local operators $e_{j\beta}^{\alpha}$ and for their restriction to the first m sites, we find the expression

$$D_{L\beta_1\cdots\beta_m}^{\alpha_1\cdots\alpha_m}(T) = \operatorname{tr}_{1\cdots m} e_{1\beta_1}^{\alpha_1} \cdots e_{m\beta_m}^{\alpha_m} D_L(T) = \left\langle e_{1\beta_1}^{\alpha_1} \cdots e_{m\beta_m}^{\alpha_m} \right\rangle_T \tag{21}$$

for the matrix elements of the density matrix.

Here we are interested in the unique (normalized) ground state $|\Psi_0\rangle$ of the system of finite even length. In the limit $T \to 0+$ the statistical operator ρ_L converges to the projector $|\Psi_0\rangle\langle\Psi_0|$ onto the ground state, and the formula (21) for the density matrix elements turns into

$$D_{L\beta_1\cdots\beta_m}^{\alpha_1\cdots\alpha_m} = \lim_{T \to 0+} D_{L\beta_1\cdots\beta_m}^{\alpha_1\cdots\alpha_m}(T) = \langle\Psi_0| e_{1\beta_1}^{\alpha_1} \cdots e_{m\beta_m}^{\alpha_m} |\Psi_0\rangle. \tag{22}$$

We shall use a trick suggested in [18] in order to express (22) entirely in terms of data related to the monodromy matrix $T(\lambda)$. Setting $\lambda = 0$ in the second equation (6), using $L_j(0) = R_{0j}(0) = P_{0j}$ (if 0 denotes the auxiliary space) and comparing both sides [13] we obtain

$$e_{j\beta}^{\alpha} = t^{j-1}(0) T_{\beta}^{\alpha}(0) t^{-j}(0). \tag{23}$$

It follows that

$$D_{L\beta_1\cdots\beta_m}^{\alpha_1\cdots\alpha_m} = \langle\Psi_0| T_{\beta_1}^{\alpha_1}(0) \cdots T_{\beta_m}^{\alpha_m}(0) t^{-m}(0) |\Psi_0\rangle. \tag{24}$$

In order to apply the techniques developed in [11] for the finite-temperature case we regularize the expression by introducing inhomogeneity parameters ξ_j, $j = 1, \ldots, m$, in the following way. Define an 'inhomogeneous density matrix'

$$D_{L\beta_1\cdots\beta_m}^{\alpha_1\cdots\alpha_m}(\xi_1, \ldots, \xi_m) = \frac{\langle\{\lambda\}| T_{\beta_1}^{\alpha_1}\left(\xi_1 - \frac{\eta}{2}\right) \cdots T_{\beta_m}^{\alpha_m}\left(\xi_m - \frac{\eta}{2}\right) |\{\lambda\}\rangle}{\langle\{\lambda\}|\{\lambda\}\rangle \prod_{j=1}^{m} \Lambda_0\left(\xi_j - \frac{\eta}{2}\right)}, \tag{25}$$

where $|\{\lambda\}\rangle$ is the (unnormalized) Bethe ansatz ground state. Then

$$D_{L\beta_1\cdots\beta_m}^{\alpha_1\cdots\alpha_m} = \lim_{\xi_1,\ldots,\xi_m \to \frac{\eta}{2}} D_{L\beta_1\cdots\beta_m}^{\alpha_1\cdots\alpha_m}(\xi_1, \ldots, \xi_m). \tag{26}$$

The expression (25) is of the same form as in the finite-temperature case considered in [10, 12] with the monodromy matrix elements obeying the same commutation relations (7). Moreover we have an auxiliary function $\mathfrak{a}(\lambda)$ which shares some of the features of the finite-temperature auxiliary function and satisfies, in particular, equation (17). The inhomogeneous density matrix can therefore be represented as a multiple integral following the same lines of reasoning as in [10]. Since the calculations are very similar we can skip all details here and present the final result.

Let $|\alpha^+|$ be the number of up-spins (or ones) in the sequence of upper indices $(\alpha_j)_{j=1}^m$ of the inhomogeneous density matrix element (25) and $|\beta^-|$ the number of down-spins (or twos) in the sequence of lower indices. The conservation of the z-component of the total spin implies that all density matrix elements with $|\alpha^+| + |\beta^-| \neq m$ must vanish. Hence, $|\beta^-| = m - |\alpha^+|$ for the non-vanishing density matrix elements. Those are conveniently labelled by two finite sequences of positive integers $(x_j)_{j=1}^{|\alpha^+|}$ and $(y_k)_{k=|\alpha^+|+1}^m$, where x_j denotes the position of the $(|\alpha^+| - j + 1)$ th up-spin in $(\alpha_j)_{j=1}^m$, and y_k denotes the position of the $(k - |\alpha^+|)$ th down-spin in $(\beta_j)_{j=1}^m$. Then

$$
\begin{aligned}
D_L{}_{\beta_1\cdots\beta_m}^{\alpha_1\cdots\alpha_m}(\xi_1,\ldots,\xi_m) = & \left[\prod_{j=1}^{|\alpha^+|}\int_{\mathcal{C}}\frac{\mathrm{d}\omega_j}{2\pi\mathrm{i}(1+\mathfrak{a}(\omega_j))}\prod_{k=1}^{x_j-1}\mathrm{sh}(\omega_j-\xi_k-\eta)\prod_{k=x_j+1}^m\mathrm{sh}(\omega_j-\xi_k)\right] \\
& \times\left[\prod_{j=|\alpha^+|+1}^m\int_{\mathcal{C}}\frac{\mathrm{d}\omega_j}{2\pi\mathrm{i}(1+\overline{\mathfrak{a}}(\omega_j))}\prod_{k=1}^{y_j-1}\mathrm{sh}(\omega_j-\xi_k+\eta)\prod_{k=y_j+1}^m\mathrm{sh}(\omega_j-\xi_k)\right] \\
& \times\frac{\det(-G(\omega_j,\xi_k))}{\prod_{1\leqslant j<k\leqslant m}\mathrm{sh}(\xi_k-\xi_j)\mathrm{sh}(\omega_j-\omega_k-\eta)},
\end{aligned}
\tag{27}
$$

where $\overline{\mathfrak{a}} = 1/\mathfrak{a}$ and where the function $G(\omega,\xi)$ has to be calculated from the linear integral equation

$$
G(\lambda,\xi) = \frac{\mathrm{sh}(\eta)}{\mathrm{sh}(\lambda-\xi)\mathrm{sh}(\lambda-\xi-\eta)} + \int_{\mathcal{C}}\frac{\mathrm{d}\omega\,G(\omega,\xi)}{2\pi(1+\mathfrak{a}(\omega))}K_\eta(\lambda-\omega).
\tag{28}
$$

The contour $\mathcal{C}$ in (27) and (28) is the same as in figure 1. Remarkably, (27) and (28) are of precisely the same form as in the finite-temperature case, the only difference being the definition of the auxiliary function $\mathfrak{a}$, equation (14). Thus, many results that were obtained for the finite-temperature case can be carried over to the finite-size case without further effort.

Performing the homogeneous limit $\xi_j \to \frac{\eta}{2}$ in (27) we obtain a multiple integral formula for the density matrix $D_L{}_{\beta_1\cdots\beta_m}^{\alpha_1\cdots\alpha_m}$. This limit was described elsewhere [12, 19]. Here we have to take into account that in the derivation of (27) and (28) we have assumed that the ξ_j lie inside $\mathcal{C}$. Thus, in order to calculate the homogeneous limit, we first have to push the contour to $\pm\frac{\eta}{2}$. It turns out that the multiple integral formula for the homogeneous density matrix is not very efficient numerically (see [8] for the finite-temperature case). For this reason and for space limitations we leave the homogeneous limit of the multiple integral as an exercise to the reader. In the next section, we shall rather proceed along the lines of the recent paper [2] where for the isotropic model the inhomogeneous formula (27) was first split into a sum over products of single integrals and where the homogeneous limit was performed only after that. To be more precise, such 'factorization' was carried out for $m = 2, 3$ and then a general formula inspired by [5] was conjectured for finite temperature but zero magnetic field.

5. Factorization for *XXX*

In the following, we restrict ourselves to the isotropic limit $\Delta \to 1$. In order to perform this limit in our formulae we have to replace η by $\mathrm{i}\epsilon$ with $\epsilon \to 0$. In a similar way, we have to rescale the spectral parameter λ in (14) and (28), the inhomogeneities, the integration variables

and the functions $\mathfrak{a}$ and G. Then

$$
D_L{}^{\alpha_1 \cdots \alpha_m}_{\beta_1 \cdots \beta_m}(\xi_1, \ldots, \xi_m) = \left[\prod_{j=1}^{|\alpha^+|} \int_{\mathcal{C}} \frac{d\omega_j}{2\pi(1 + \mathfrak{a}(\omega_j))} \prod_{k=1}^{x_j - 1} (\omega_j - \xi_k - i) \prod_{k=x_j+1}^{m} (\omega_j - \xi_k) \right]
$$

$$
\times \left[\prod_{j=|\alpha^+|+1}^{m} \int_{\mathcal{C}} \frac{d\omega_j}{2\pi(1 + \overline{\mathfrak{a}}(\omega_j))} \prod_{k=1}^{y_j - 1} (\omega_j - \xi_k + i) \prod_{k=y_j+1}^{m} (\omega_j - \xi_k) \right]
$$

$$
\times \frac{\det G(\omega_j, \xi_k)}{\prod_{1 \leqslant j < k \leqslant m} (\xi_k - \xi_j)(\omega_j - \omega_k - i)}. \tag{29}
$$

The rescaled auxiliary function $\mathfrak{a}$ satisfies the nonlinear integral equation

$$
\ln \mathfrak{a}(\lambda) = -2i\Phi + L \ln \left(\frac{\lambda - \frac{i}{2}}{\lambda + \frac{i}{2}} \right) - \int_{\mathcal{C}} \frac{d\omega}{\pi} \frac{\ln(1 + \mathfrak{a}(\omega))}{1 + (\lambda - \omega)^2}, \tag{30}
$$

and $\overline{\mathfrak{a}} = 1/\mathfrak{a}$. The contour now surrounds the real axis counterclockwise slightly below $\mathrm{Im}\,\lambda = \frac{1}{2}$ and slightly above $\mathrm{Im}\,\lambda = -\frac{1}{2}$. The rescaled G in the *XXX* limit is defined by an integral equation on the same contour which reads

$$
G(\lambda, \xi) + \frac{1}{(\lambda - \xi)(\lambda - \xi - i)} = \int_{\mathcal{C}} \frac{d\omega}{\pi(1 + \mathfrak{a}(\omega))} \frac{G(\omega, \xi)}{1 + (\lambda - \omega)^2}. \tag{31}
$$

For the following it is important to note that (29) and (31) are exactly of the same form as in the finite-temperature case [2], where (for $m = 2, 3$) (31) was used in order to factorize (29). The argument did not depend on the form of $\mathfrak{a}$ and therefore applies here in exactly the same way. We just have to replace the finite-temperature auxiliary function used in [2] by the finite-size auxiliary function (30).

Let us review the results of [2]. It was shown that the inhomogeneous density matrix for m up to 3 can be expressed in terms of functions defined by single integrals. The most important one is

$$
\psi(\xi_1, \xi_2) = \int_{\mathcal{C}} \frac{d\omega \, G(\omega, \xi_1)}{\pi(1 + \mathfrak{a}(\omega))} \frac{1}{(\omega - \xi_2)(\omega - \xi_2 - i)}. \tag{32}
$$

We suggest (see the conjecture below) that this is the only transcendental function needed in the description of the inhomogeneous density matrix for arbitrary m and vanishing twist angle $\Phi = 0$, and that in this case, the length dependence of the density matrix enters through $\psi(\xi_1, \xi_2)$ alone. If we want to consider nonzero Φ we have to deal with another family of functions

$$
\phi_j(\xi) = \int_{\mathcal{C}} \frac{d\omega \, \omega^{j-1} G(\omega, \xi)}{\pi(1 + \mathfrak{a}(\omega))}, \qquad j \in \mathbb{N} \tag{33}
$$

which where called moments in [2].

For a compact notation of our final formulae it turns out to be useful to introduce certain combinations of the moments with rational functions. We first of all note that in the thermodynamic limit for zero twist angle the moments turn into polynomials in ξ of order $j - 1$,

$$
\lim_{1/L \to 0} \lim_{\Phi \to 0} \phi_j(\xi) = \phi_j^{(0)}(\xi) = (-i\partial_k)^{j-1} \frac{2 \, e^{ik\xi}}{1 + e^k} |_{k=0}. \tag{34}
$$

The 'normalized moments',

$$
\varphi_j(\xi) = \phi_j(\xi) - \phi_j^{(0)}(\xi), \tag{35}
$$

then vanish for $1/L$, $\Phi \to 0$. We use them to define the symmetric combinations

$$\Delta_n(\xi_1, \ldots, \xi_n) = \frac{\det(\varphi_j(\xi_k))|_{j,k=1,\ldots,n}}{\prod_{1 \leqslant j < k \leqslant n} \xi_{kj}}, \tag{36}$$

where the shorthand notation $\xi_{kj} = \xi_k - \xi_j$ was employed. The first moment φ_1 is exceptional among the φ_j in that it becomes trivial even for finite length if only the twist angle vanishes,

$$\lim_{\Phi \to 0} \varphi_1(\xi) = 0. \tag{37}$$

It follows that

$$\lim_{\Phi \to 0} \Delta_j(\xi) = 0, \qquad \text{for all} \quad j \in \mathbb{N}. \tag{38}$$

Instead of $\psi(\xi_1, \xi_2)$ we shall use the closely related expression

$$\gamma(\xi_1, \xi_2) = [1 + (\xi_1 - \xi_2)^2]\psi(\xi_1, \xi_2) - 1 \tag{39}$$

in terms of which our final formulae look neater. We also define

$$\gamma_0(\xi_1, \xi_2) = \lim_{\Phi \to 0} \gamma(\xi_1, \xi_2). \tag{40}$$

All density matrix elements for $m = 1, 2, 3$ can be written in terms of these functions. A complete list can be found in the appendix of [2] where the functions $\gamma(\xi_j, \xi_k)$ and $\Delta_n(\xi_1, \ldots, \xi_n)$ have to be inserted according to our definitions above. To give examples let us only recall the expressions for the emptiness formation probabilities here,

$$D_{L\,11}^{\,11}(\xi_1, \xi_2) = \frac{1}{4} - \frac{1}{12}\gamma(\xi_1, \xi_2) + \frac{1}{4}(\Delta_1(\xi_1) + \Delta_1(\xi_2)) + \frac{1}{6}\Delta_2(\xi_1, \xi_2), \tag{41a}$$

$$\begin{aligned} D_{L\,111}^{\,111}(\xi_1, \xi_2, \xi_3) = {} & \frac{1}{24} + \frac{1 - \xi_{13}\xi_{23}}{24\xi_{13}\xi_{23}}\gamma(\xi_1, \xi_2) \\ & + \frac{1 + 5\xi_{12}\xi_{13}}{40\xi_{12}\xi_{13}}\Delta_1(\xi_1) + \frac{1 + 2\xi_{13}\xi_{23}}{24\xi_{13}\xi_{23}}\Delta_2(\xi_1, \xi_2) + \frac{1}{60}\Delta_3(\xi_1, \xi_2, \xi_3) \\ & - \frac{3 + 2\xi_{12}^2 + 5\xi_{13}\xi_{23}}{120\xi_{13}\xi_{23}}\gamma(\xi_1, \xi_2)\Delta_1(\xi_3) + \text{cyclic perms.} \end{aligned} \tag{41b}$$

In the untwisted limit (38) applies and our result reduces to

$$D_{L\,11}^{\,11}(\xi_1, \xi_2) = \frac{1}{4} - \frac{1}{12}\gamma_0(\xi_1, \xi_2), \tag{42a}$$

$$D_{L\,111}^{\,111}(\xi_1, \xi_2, \xi_3) = \frac{1}{24} + \frac{1 - \xi_{13}\xi_{23}}{24\xi_{13}\xi_{23}}\gamma_0(\xi_1, \xi_2) + \text{cyclic perms.} \tag{42b}$$

Note that the only effect of taking the limit $1/L \to 0$ here is that the function $\gamma_0(\xi_1, \xi_2)$ changes into its limiting form

$$\lim_{1/L \to 0} \gamma_0(\xi_1, \xi_2) = 2[1 + (\xi_1 - \xi_2)^2]\mathcal{K}(\xi_1 - \xi_2) - 1, \tag{43}$$

where

$$\mathcal{K}(x) = \mathrm{i}\,\partial_x \ln\left[\frac{\Gamma\left(\frac{1}{2} + \frac{\mathrm{i}x}{2}\right)\Gamma\left(1 - \frac{\mathrm{i}x}{2}\right)}{\Gamma\left(\frac{1}{2} - \frac{\mathrm{i}x}{2}\right)\Gamma\left(1 + \frac{\mathrm{i}x}{2}\right)}\right]. \tag{44}$$

As in the temperature case a similar statement holds true for all density matrix elements for $m = 1, 2$. The rational prefactors of $\gamma_0(\xi_j, \xi_k)$ are the same as in the thermodynamic limit. For

this reason it was conjectured in [2] for the temperature case that the exponential formula for general m obtained in [5] holds also for finite temperature. Further evidence for this conjecture was supplied by the comparison of high-temperature expansion data for the multiple integrals and for the conjectured exponential formula for $m = 3, 4$. Regarding our results described above it seems likely that the scope of the exponential formula is even wider and that it also holds in the finite-length case under consideration. Let us briefly recall how it looks like.

In order to obtain a convenient description of all density matrix elements we shall resort to a notation that we borrowed from [4][1]. We arrange them into a column vector $h_m \in (\mathbb{C}^2)^{\otimes 2m}$ with coordinates labelled by $+, -$ instead of $1, 2$ according to the rule,

$$h_m^{\varepsilon_1,\ldots,\varepsilon_m,\bar{\varepsilon}_m,\ldots,\bar{\varepsilon}_1}(\lambda_1,\ldots,\lambda_m) = D_{L(3+\bar{\varepsilon}_1)/2,\ldots,(3+\bar{\varepsilon}_m)/2}^{(3-\varepsilon_1)/2,\ldots,(3-\varepsilon_m)/2}(\xi_1,\ldots,\xi_m) \cdot \prod_{j=1}^{m}(-\bar{\varepsilon}_j), \tag{45}$$

where $\lambda_j = -\mathrm{i}\xi_j$ for $j = 1,\ldots,m$.

Conjecture. *The density matrix of a finite sub-chain of length m of the XXX chain of finite length L is determined by the vector*

$$h_m(\lambda_1,\ldots,\lambda_m) = \frac{1}{2^m}\,\mathrm{e}^{\Omega_m(\lambda_1,\ldots,\lambda_m)}\mathbf{s}_m, \qquad \mathbf{s}_m = \prod_{j=1}^{m} s_{j,\bar{j}}, \tag{46}$$

$$\Omega_m(\lambda_1,\ldots,\lambda_m) = \frac{(-1)^{(m-1)}}{4}\int\int \frac{\mathrm{d}\mu_1}{2\pi\mathrm{i}}\frac{\mathrm{d}\mu_2}{2\pi\mathrm{i}}\frac{\gamma_0(\mathrm{i}\mu_1,\mathrm{i}\mu_2)(\mu_1 - \mu_2)}{[1 - (\mu_1 - \mu_2)^2]^2}$$
$$\times \mathrm{tr}_{\mu_{1,2},2,2}\left\{T\left(\frac{\mu_1 + \mu_2}{2};\lambda_1,\ldots,\lambda_m\right) \otimes [T(\mu_1;\lambda_1,\ldots,\lambda_m)\right.$$
$$\left. \otimes T(\mu_2;\lambda_1,\ldots,\lambda_m)\mathcal{P}^-]\right\}, \tag{47}$$

through (45). By the integral over μ_1, μ_2 it is meant to take the residues at the poles $\lambda_1, \ldots, \lambda_m$ of the integrand.

For the notation we are referring to [5][2]: the vector $s = \binom{1}{0} \otimes \binom{0}{1} - \binom{0}{1} \otimes \binom{1}{0}$ is the spin singlet in $\mathbb{C}^2 \otimes \mathbb{C}^2$. The vector spaces in $(\mathbb{C}^2)^{\otimes 2m}$ are numbered in the order $1, 2, \ldots, n, \bar{n}, \overline{n-1}, \ldots, \bar{1}$. This defines $\mathbf{s}_m$. $\mathcal{P}^-$ is the projector onto the one-dimensional subspace of $\mathbb{C}^2 \otimes \mathbb{C}^2$ spanned by s.

In order to define the transfer matrices in the integrand in (47) we first of all introduce an L-matrix $L(\lambda) \in U(\mathfrak{sl}_2) \otimes \mathrm{End}\,\mathbb{C}^2$,

$$L(\lambda) = \frac{\rho(\lambda, d)}{2\lambda + d}(2\lambda + 1 + \Sigma^\alpha \otimes \sigma^\alpha), \tag{48}$$

where the $\Sigma^\alpha \in \mathfrak{sl}_2$ are a basis satisfying $[\Sigma^\alpha, \Sigma^\beta] = 2\mathrm{i}\varepsilon^{\alpha\beta\gamma}\Sigma^\gamma$, where d is determined by the Casimir element through $d^2 = (\Sigma^\alpha)^2 + 1$ and where $\rho(\lambda, d)$ satisfies the functional relation

$$\rho(\lambda, d)\rho(\lambda - 1, d) = \frac{2 - 2\lambda - d}{2\lambda - d} \tag{49}$$

---

[1] This definition was first introduced in [3] and later modified in [4].
[2] In fact, the only difference between our formulae (46) and (47) and the result of [5] is in the function γ_0. In [5] a function ω was used which is related to γ_0 by

$$\omega(\lambda_1 - \lambda_2) = \lim_{1/L \to 0} \frac{\gamma_0(\mathrm{i}\lambda_1, \mathrm{i}\lambda_2)}{2(1 - (\lambda_1 - \lambda_2)^2)}.$$

(for more details see [5]). Then, for integer z, the 'transfer matrices'

$$\text{tr}_z T(\lambda; \lambda_1, \ldots, \lambda_n) = \text{tr}_z L_{\bar{1}}(\lambda - \lambda_1 - 1) \cdots L_{\bar{n}}(\lambda - \lambda_n - 1) L_n(\lambda - \lambda_n) \cdots L_1(\lambda - \lambda_1) \quad (50)$$

entering (47) are defined by substituting the irreducible representation of $U(\mathfrak{sl}_2)$ of dimension z into the definition (48) of the L-matrices. For non-integer z this can be analytically continued into the complex plane.

6. A numerical case study

Finally we would like to demonstrate that the formulae obtained above are numerically efficient, at least for small m. The examples we will be focusing on are the zz-correlation functions $\langle \sigma_1^z \sigma_2^z \rangle$ and $\langle \sigma_1^z \sigma_3^z \rangle$ as functions of the chain length L in the untwisted case $\Phi = 0$. For these it is sufficient to know the emptiness formation probability for $m = 2, 3$, since

$$\langle \sigma_1^z \sigma_2^z \rangle = 4 D_L{}_{11}^{11} - 1, \qquad \langle \sigma_1^z \sigma_3^z \rangle = 8 D_L{}_{111}^{111} - 8 D_L{}_{11}^{11} + 1. \quad (51)$$

Hence, we have to perform the homogeneous limit $\xi_j \to \frac{i}{2}$ in (42), yielding

$$\langle \sigma_1^z \sigma_2^z \rangle = -\frac{1}{3} \gamma_0 \left(\frac{i}{2}, \frac{i}{2} \right) = \frac{1}{3} - \frac{1}{3} \psi \left(\frac{i}{2}, \frac{i}{2} \right), \quad (52a)$$

$$\langle \sigma_1^z \sigma_3^z \rangle = -\frac{1}{3} \gamma_0 \left(\frac{i}{2}, \frac{i}{2} \right) - \frac{1}{6} \gamma_{0,xx} \left(\frac{i}{2}, \frac{i}{2} \right) + \frac{1}{3} \gamma_{0,xy} \left(\frac{i}{2}, \frac{i}{2} \right)$$

$$= \frac{1}{3} - \frac{4}{3} \psi \left(\frac{i}{2}, \frac{i}{2} \right) - \frac{1}{6} \psi_{xx} \left(\frac{i}{2}, \frac{i}{2} \right) + \frac{1}{3} \psi_{xy} \left(\frac{i}{2}, \frac{i}{2} \right), \quad (52b)$$

where we denote derivatives with respect to the first and second argument by subscripts x and y, respectively.

In order to calculate the functions ψ, ψ_{xx} and ψ_{xy} on a computer we switch to the $\mathfrak{b}\bar{\mathfrak{b}}$-formulation [8, 21] mentioned in section 3. For real x we define $\mathfrak{b}(x) = \mathfrak{a}\left(x + \frac{i}{2} \right)$ and $\bar{\mathfrak{b}}(x) = \bar{\mathfrak{a}}\left(x - \frac{i}{2} \right)$. Then [21]

$$\ln \mathfrak{b}(x) = L \ln(\text{th}(\pi x/2)) + \int_{-\infty}^{\infty} \frac{dy}{2\pi} \mathcal{K}(x - y) \ln(1 + \mathfrak{b}(y))$$

$$- \int_{-\infty}^{\infty} \frac{dy}{2\pi} \mathcal{K}(x - y + i - i0) \ln(1 + \bar{\mathfrak{b}}(y)), \quad (53a)$$

$$\ln \bar{\mathfrak{b}}(x) = L \ln(\text{th}(\pi x/2)) + \int_{-\infty}^{\infty} \frac{dy}{2\pi} \mathcal{K}(x - y) \ln(1 + \bar{\mathfrak{b}}(y))$$

$$- \int_{-\infty}^{\infty} \frac{dy}{2\pi} \mathcal{K}(x - y - i + i0) \ln(1 + \mathfrak{b}(y)), \quad (53b)$$

where $\mathcal{K}(x)$ is defined by (44). The function ψ and its derivatives can be expressed in terms of $\mathfrak{b}$ and $\bar{\mathfrak{b}}$. For this purpose, we also have to adapt the form of the function $G(\lambda, \xi)$. Following [8] we define $g_\xi^{(\pm)}(x) = \pm G\left(x \pm \frac{i}{2}, \xi \right)$. These functions satisfy the linear integral equations:

$$g_\xi^{(+)}(x) = \frac{\pi}{\text{ch}(\pi(\xi - x))} + \int_{-\infty}^{\infty} \frac{dy \, g_\xi^{(+)}(y)}{2\pi(1 + \mathfrak{b}^{-1}(y))} \mathcal{K}(x - y)$$

$$- \int_{-\infty}^{\infty} \frac{dy \, g_\xi^{(-)}(y)}{2\pi(1 + \bar{\mathfrak{b}}^{-1}(y))} \mathcal{K}(x - y + i - i0), \quad (54a)$$

$$g_\xi^{(-)}(x) = \frac{\pi}{\mathrm{ch}(\pi(\xi-x))} + \int_{-\infty}^{\infty} \frac{\mathrm{d}y\, g_\xi^{(-)}(y)}{2\pi(1+\overline{\mathfrak{b}}^{-1}(y))} \mathcal{K}(x-y)$$

$$- \int_{-\infty}^{\infty} \frac{\mathrm{d}y\, g_\xi^{(+)}(y)}{2\pi(1+\mathfrak{b}^{-1}(y))} \mathcal{K}(x-y-\mathrm{i}+\mathrm{i}0). \tag{54b}$$

Using $\mathfrak{b}, \overline{\mathfrak{b}}$ and $g_\xi^{(\pm)}$ we can express the function $\psi(\xi_1, \xi_2)$ as

$$\psi(\xi_1,\xi_2) = 2\mathcal{K}(\xi_1-\xi_2) + \int_{-\infty}^{\infty} \frac{\mathrm{d}x}{\mathrm{ch}(\pi(\xi_2-x))} \left[\frac{g_{\xi_1}^{(+)}(x)}{1+\mathfrak{b}^{-1}(x)} + \frac{g_{\xi_1}^{(-)}(x)}{1+\overline{\mathfrak{b}}^{-1}(x)} \right]. \tag{55}$$

This formulation is now convenient for the numerical evaluation of the zz-correlation functions (52) for which we need $\psi\left(\frac{\mathrm{i}}{2}, \frac{\mathrm{i}}{2}\right)$, $\psi_{xx}\left(\frac{\mathrm{i}}{2}, \frac{\mathrm{i}}{2}\right)$ and $\psi_{xy}\left(\frac{\mathrm{i}}{2}, \frac{\mathrm{i}}{2}\right)$. For the expansion of the kernel function we can use

$$\mathcal{K}(x) = 2\sum_{k=0}^{\infty} (-1)^k \zeta_a(2k+1) x^{2k}, \tag{56}$$

where $\zeta_a(x) = \sum_{k=1}^{\infty} (-1)^{k+1}/k^x$ is the alternating zeta series[3]. Then

$$\psi\left(\frac{\mathrm{i}}{2}, \frac{\mathrm{i}}{2}\right) = 4\ln 2 + \int_{-\infty}^{\infty} \frac{\mathrm{i}\,\mathrm{d}x}{\mathrm{sh}(\pi(x+\mathrm{i}0))} \left[\frac{g_{\mathrm{i}/2}^{(+)}(x)}{1+\mathfrak{b}^{-1}(x)} + \frac{g_{\mathrm{i}/2}^{(-)}(x)}{1+\overline{\mathfrak{b}}^{-1}(x)} \right],$$

$$\psi_{xy}\left(\frac{\mathrm{i}}{2}, \frac{\mathrm{i}}{2}\right) = 6\zeta(3) + \int_{-\infty}^{\infty} \frac{\mathrm{d}x\, \mathrm{i}\pi\,\mathrm{ch}(\pi x)}{\mathrm{sh}^2(\pi(x+\mathrm{i}0))} \left[\frac{g_{\mathrm{i}/2}^{(+)\prime}(x)}{1+\mathfrak{b}^{-1}(x)} + \frac{g_{\mathrm{i}/2}^{(-)\prime}(x)}{1+\overline{\mathfrak{b}}^{-1}(x)} \right], \tag{57}$$

$$\psi_{xx}\left(\frac{\mathrm{i}}{2}, \frac{\mathrm{i}}{2}\right) = -6\zeta(3) + \int_{-\infty}^{\infty} \frac{\mathrm{i}\,\mathrm{d}x}{\mathrm{sh}(\pi(x+\mathrm{i}0))} \left[\frac{g_{\mathrm{i}/2}^{(+)\prime\prime}(x)}{1+\mathfrak{b}^{-1}(x)} + \frac{g_{\mathrm{i}/2}^{(-)\prime\prime}(x)}{1+\overline{\mathfrak{b}}^{-1}(x)} \right],$$

where the primes denote derivatives with respect to ξ. Using (54) and (57) in (52) we calculated the nearest and next-to-nearest neighbour zz-correlators numerically. The nonlinear integral equations (53) as well as the linear integral equations (54) were solved iteratively in Fourier space. The derivatives of $g_\xi^{(\pm)}$ with respect to ξ were computed by solving the integral equations obtained from (54) by taking the derivatives with respect to ξ.

Figure 2 shows the nearest neighbour correlator and figure 3 the next-to-nearest neighbour correlator. Since our model represents an antiferromagnet the former must be negative and the latter positive. The weakening of the correlation with growing length can be attributed to what is called 'quantum frustration' in condensed matter physics. Let us illustrate this notion with an example. The (unnormalized) ground states of the *XXX* chain of length 2 and 4, respectively, are

$$|gs\rangle_2 = \underbrace{|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle}_{\text{Néel}},$$

$$|gs\rangle_4 = \underbrace{2|\downarrow\uparrow\downarrow\uparrow\rangle + 2|\uparrow\downarrow\uparrow\downarrow\rangle}_{\text{Néel}} - \underbrace{|\downarrow\downarrow\uparrow\uparrow\rangle - |\uparrow\downarrow\downarrow\uparrow\rangle - |\uparrow\uparrow\downarrow\downarrow\rangle - |\downarrow\uparrow\uparrow\downarrow\rangle}_{\text{QM frustration}}. \tag{58}$$

The states with alternating up and down spins on consecutive sites are called Néel states. They are a 'classical caricature' of an antiferromagnet. The zz-correlators in a Néel state are $\langle \sigma_1^z \sigma_{n+1}^z \rangle = (-1)^n$ and realize 'perfect antiferromagnetic order'. Such type of order is realized in the ground state of the *XXX* chain only for $L = 2$, where the correlations look

---

[3] For $\mathrm{Re}\, x > 1$ the Riemann zeta function $\zeta(x)$ and $\zeta_a(x)$ are related by $\zeta_a(x) = (1-2^{1-x})\zeta(x)$.
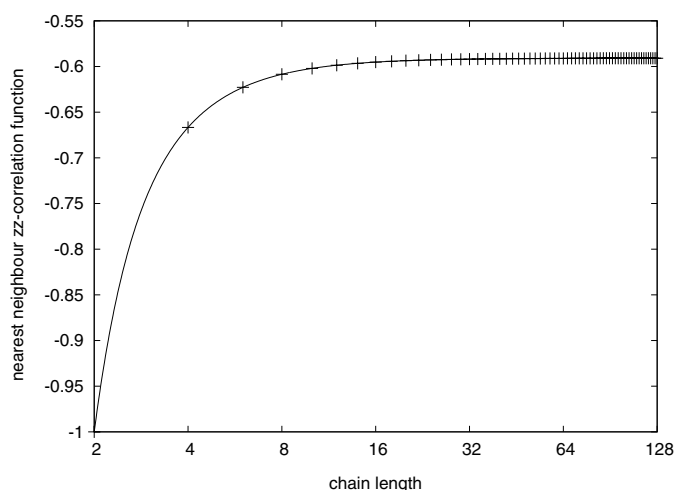
Figure 2. Nearest neighbour zz-correlation function for chains of even length L; solid curve represents the analytic continuation to arbitrary real and positive L as defined by our integral representation.
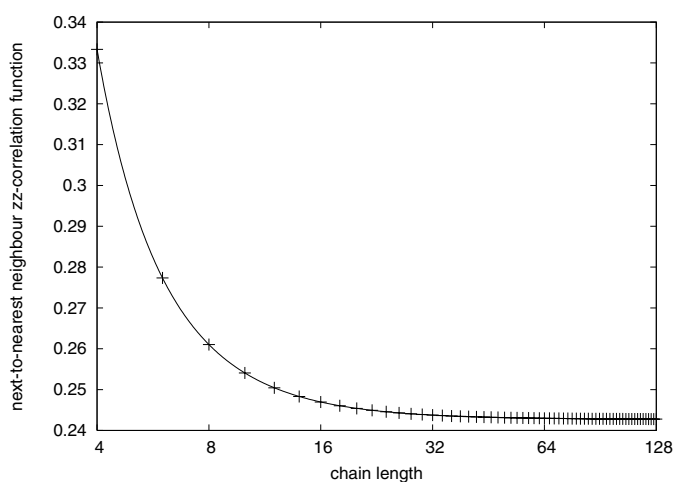

Figure 3. Next-to-nearest neighbour zz-correlation function for chains of even length L; solid curve represents the analytic continuation to arbitrary real and positive L as defined by our integral representation.

like that in the classical case (see figure 2) and where the next-to-nearest neighbour correlator is not defined. For $L = 4$, as can be seen from the ground-state wavefunction (58), there is a certain probability to have parallel spins on neighbouring sites and antiparallel spins on next-to-nearest neighbour sites. This reduces the correlations in both cases. For growing chain length the 'Néel order' is even more frustrated, e.g. three or four parallel spins appear, and the correlations are further reduced, which explains the monotonous behaviour of our curves in figures 2 and 3.

Table 1. zz-correlators as functions of the system size.

L	$\langle \sigma_1^z \sigma_2^z \rangle$	$\langle \sigma_1^z \sigma_3^z \rangle$
2	$-1.000\,000\,000\,000\,00$	–
4	$-0.666\,666\,666\,666\,67$	$0.333\,333\,333\,333\,33$
8	$-0.608\,515\,568\,156\,20$	$0.261\,037\,205\,348\,39$
16	$-0.595\,191\,363\,384\,73$	$0.246\,965\,841\,679\,98$
32	$-0.591\,938\,643\,289\,56$	$0.243\,749\,379\,898\,65$
64	$-0.591\,131\,278\,861\,52$	$0.242\,973\,291\,835\,05$
128	$-0.590\,929\,940\,117\,45$	$0.242\,782\,231\,277\,53$
256	$-0.590\,879\,657\,821\,93$	$0.242\,734\,814\,832\,57$
512	$-0.590\,867\,093\,857\,81$	$0.242\,723\,006\,016\,42$
1024	$-0.590\,863\,953\,834\,99$	$0.242\,720\,060\,216\,44$
∞	$-0.590\,862\,907\,413\,26$	$0.242\,719\,079\,825\,74$

It follows by inspection of equation (53) that $\mathfrak{b}(x)$ and $\overline{\mathfrak{b}}(x)$ vanish in the thermodynamic limit $L \to \infty$. Hence, the integrals in (57) all vanish and $\psi\left(\frac{i}{2}, \frac{i}{2}\right) = 4\ln 2$, $\psi_{xy}\left(\frac{i}{2}, \frac{i}{2}\right) = 6\zeta(3)$, $\psi_{xx}\left(\frac{i}{2}, \frac{i}{2}\right) = -6\zeta(3)$. Inserting this into (52) we obtain

$$\lim_{L\to\infty} \langle \sigma_1^z \sigma_2^z \rangle = \tfrac{1}{3} - \tfrac{4}{3}\ln 2, \qquad \lim_{L\to\infty} \langle \sigma_1^z \sigma_3^z \rangle = \tfrac{1}{3} - \tfrac{16}{3}\ln 2 + 3\zeta(3). \qquad (59)$$

The first equation is a corollary to Hulthén's classical result [14] on the ground-state energy per site of the *XXX* chain, and the second one is a well-known result due to Takahashi [25] which was reproduced from the multiple integral formula of Jimbo *et al* [15] by Boos and Korepin [7]. Here we have calculated the correlation functions for finite chain length as correction to the asymptotic values (59). The zz-correlators for $L = 4$, far away from these asymptotic values, can be easily obtained from the ground-state wavefunction $|gs\rangle_4$ in (58), $\langle \sigma_1^z \sigma_2^z \rangle = -\frac{2}{3}$ and $\langle \sigma_1^z \sigma_3^z \rangle = \frac{1}{3}$. It is remarkable that these values are reproduced from our integral equations to 13 digits precision without too much effort (see table 1).

7. Conclusions

We have obtained a multiple integral formula (27) for the zero-temperature limit of the density matrix of a finite segment of the *XXZ* chain which holds for every even chain length L and is again of the same form as the formerly known formula for finite temperature but infinite length. The multiple integrals are 'parameterized' by a pair of functions $\mathfrak{a}(\lambda)$, $G(\lambda, \xi)$ which fix their physical meaning. For one such pair we obtain the finite-temperature density matrix for another pair the ground-state density matrix for the finite chain, the only difference being the driving term in the nonlinear integral equation (14) for $\mathfrak{a}(\lambda)$. In the thermodynamic limit for vanishing twist angle (the zero-temperature limit for vanishing magnetic field) the integrands in the multiple integrals turn into explicit functions and the formulae of Jimbo *et al* [15, 16] are recovered.

Even the linear integral equations for $G(\lambda, \xi)$ are of the same form in the temperature case and in the finite-length case. Since only this form was relevant for the reduction of the multiple integrals to sums over products of single integrals (the 'factorization') in the finite-temperature case [2], a similar factorized form of the short-range correlations is valid for finite length and the conjecture formulated for the general finite-temperature case in [2] is likely to hold in the finite-length case as well (see (46)). The phenomenon of factorization of correlation functions, first observed in [7] and rather well understood in the thermodynamic

limit for zero temperature and vanishing external field by now [5], may turn out to be valid in a much broader context (compare the discussion in the summary of [9]) and may even turn out to be a general characteristic of quantum integrable models related to the Yang–Baxter equation.

In this work, we have concentrated on the density matrix, since we wanted to test if the factorization scheme of [2] also works in the finite-length case. We have seen that this is indeed the case. Concerning the multiple integral representation we have no doubt that similar formulae as derived for the two-point functions [10] and for a generating function of the zz-correlation functions [11] for finite-temperature in the thermodynamic limit also hold for finite length. It will be interesting to compare the formulae for the generating function obtainable by using the auxiliary function $\mathfrak{a}$ and our function G with the result of [17], where another multiple integral for the finite-length system was derived.

Acknowledgments

References

[1] Baxter R J 1982 *Exactly Solved Models in Statistical Mechanics* (London: Academic)
[2] Boos H, Göhmann F, Klümper A and Suzuki J 2006 Factorization of multiple integrals representing the density matrix of a finite segment of the Heisenberg spin chain *J. Stat. Mech.* P04001
[3] Boos H, Jimbo M, Miwa T, Smirnov F and Takeyama Y 2005 A recursion formula for the correlation functions of an inhomogeneous *XXX* model *Algebra Anal.* **17** 115
[4] Boos H, Jimbo M, Miwa T, Smirnov F and Takeyama Y 2006 Algebraic representation of correlation functions in integrable spin chains *Ann. Henri Poincaré* **7** 1395
[5] Boos H, Jimbo M, Miwa T, Smirnov F and Takeyama Y 2006 Density matrix of a finite sub-chain of the Heisenberg anti-ferromagnet *Lett. Math. Phys.* **75** 201
[6] Boos H, Jimbo M, Miwa T, Smirnov F and Takeyama Y 2006 Reduced qKZ equation and correlation functions of the *XXZ* model *Commun. Math. Phys.* **261** 245
[7] Boos H E and Korepin V E 2001 Quantum spin chains and Riemann zeta function with odd arguments *J. Phys. A: Math. Gen.* **34** 5311
[8] Bortz M and Göhmann F 2005 Exact thermodynamic limit of short range correlation functions of the antiferromagnetic *XXZ* chain at finite temperatures *Eur. Phys. J.* B **46** 399
[9] Boukraa S, Hassani S, Maillard J-M, McCoy B M, Orrick W P and Zenine N 2007 Holonomy of the Ising model form factors *J. Phys. A: Math. Theor.* **40** 75
[10] Göhmann F, Hasenclever N P and Seel A 2005 The finite temperature density matrix and two-point correlations in the antiferromagnetic *XXZ* chain *J. Stat. Mech.* P10015
[11] Göhmann F, Klümper A and Seel A 2004 Integral representations for correlation functions of the *XXZ* chain at finite temperature *J. Phys. A: Math. Gen.* **37** 7625
[12] Göhmann F, Klümper A and Seel A 2005 Integral representation of the density matrix of the *XXZ* chain at finite temperature *J. Phys. A: Math. Gen.* **38** 1833
[13] Göhmann F and Korepin V E 2000 Solution of the quantum inverse problem *J. Phys. A: Math. Gen.* **33** 1199
[14] Hulthén L 1938 Über das Austauschproblem eines Kristalles *Arkiv för Matematik, Astronomi och Fysik* A **26** A1
[15] Jimbo M, Miki K, Miwa T and Nakayashiki A 1992 Correlation functions of the *XXZ* model for $\Delta < -1$ *Phys. Lett.* A **168** 256
[16] Jimbo M and Miwa T 1996 Quantum KZ equation with $|q| = 1$ and correlation functions of the *XXZ* model in the gapless regime *J. Phys. A: Math. Gen.* **29** 2923
[17] Kitanine N, Maillet J M, Slavnov N A and Terras V 2005 Master equation for spin–spin correlation functions of the *XXZ* chain *Nucl. Phys.* B **712** 600

[18] Kitanine N, Maillet J M and Terras V 1999 Form factors of the *XXZ* Heisenberg spin-$\frac{1}{2}$ finite chain *Nucl. Phys. B* **554** 647

[19] Kitanine N, Maillet J M and Terras V 2000 Correlation functions of the *XXZ* Heisenberg spin-$\frac{1}{2}$ chain in a magnetic field *Nucl. Phys. B* **567** 554

[20] Klümper A and Batchelor M T 1990 An analytic treatment of finite-size corrections of the spin-1 antiferromagnetic *XXZ* chain *J. Phys. A: Math. Gen.* **23** L189

[21] Klümper A, Batchelor M T and Pearce P A 1991 Central charges of the 6- and 19-vertex models with twisted boundary conditions *J. Phys. A: Math. Gen.* **24** 3111

[22] Korepin V E, Bogoliubov N M and Izergin A G 1993 *Quantum Inverse Scattering Method and Correlation Functions* (Cambridge: Cambridge University Press)

[23] Suzuki M 1985 Transfer-matrix method and Monte Carlo simulation in quantum spin systems *Phys. Rev. B* **31** 2957

[24] Suzuki M and Inoue M 1987 The ST-transformation approach to analytic solutions of quantum systems: I. General formulations and basic limit theorems *Prog. Theor. Phys.* **78** 787

[25] Takahashi M 1977 Half-filled Hubbard model at low temperature *J. Phys. C: Solid State Phys.* **10** 1289