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Integral representation of the density matrix of the XXZ chain at finite temperatures

Frank Göhmann, Andreas Klümper and Alexander Seel

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

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

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Abstract

We present an integral formula for the density matrix of a finite segment of the infinitely long spin-$\frac{1}{2}$ XXZ chain. This formula is valid for any temperature and any longitudinal magnetic field.

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1. Introduction

A system which is a part of a larger system and interacts with its other parts cannot be in a pure quantum state and must be described by a density matrix [19]. The calculation of the density matrix involves taking the trace over all those degrees of freedom of the larger system which do not belong to the subsystem we are interested in and, in the thermodynamic limit, when the subsystem stays finite, but the large system becomes infinitely large, is usually rather hard. One of the few examples where a density matrix could be calculated for an interacting system is the antiferromagnetic spin-$\frac{1}{2}$ XXZ chain with the Hamiltonian

$$H_{\mathrm{XXZ}} = J \sum_{j=1}^{L} \big(\sigma_{j-1}^x \sigma_j^x + \sigma_{j-1}^y \sigma_j^y + \Delta\big(\sigma_{j-1}^z \sigma_j^z - 1\big)\big) \tag{1}$$

acting on the tensor product of spaces of states of L spins $\frac{1}{2}$. The σ^α, $\alpha = x, y, z$, in (1) are the Pauli matrices and $J > 0$ and $\Delta > -1$ are two real parameters, the exchange interaction and the exchange anisotropy.

In [8, 9, 14] integral formulae for the zero temperature density matrix elements of a segment of length m of the infinite chain were obtained. Since the expectation value of any operator acting on a segment of length m can be expressed in terms of the density matrix elements (see equation (13)), the density matrix enables one, in particular, to calculate the correlations of local observables (for recent developments see [13]). This is the reason why the density matrix elements were called 'elementary blocks of correlation functions' in [8, 9, 14] and also is the actual reason why we got interested in the subject. In fact, much recent progress in the calculation of short-range correlations for the XXZ chain [2, 3, 5, 10, 11, 20, 26] originates in the integral representation of the density matrix obtained in [8, 9, 14].

Below we generalize the formulae first obtained in [8, 9, 14] to finite temperatures. It turns out that the same means that where successfully applied in the calculation of a generating function of the S^z–S^z correlation functions at finite temperatures in [7] also work for the density matrix. Namely we may combine algebraic Bethe ansatz techniques for the calculation of matrix elements [14, 17, 18, 21] with the quantum transfer matrix approach to the thermodynamics of quantum spin chains [15, 16, 22, 25].

2. The quantum transfer matrix

All properties of the XXZ chain can be derived from the well-known trigonometric solution

$$R(\lambda, \mu) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & b(\lambda, \mu) & c(\lambda, \mu) & 0 \\ 0 & c(\lambda, \mu) & b(\lambda, \mu) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{2}$$

of the Yang–Baxter equation, where

$$b(\lambda, \mu) = \frac{\operatorname{sh}(\lambda - \mu)}{\operatorname{sh}(\lambda - \mu + \eta)}, \qquad c(\lambda, \mu) = \frac{\operatorname{sh}(\eta)}{\operatorname{sh}(\lambda - \mu + \eta)}. \tag{3}$$

This R-matrix not only generates Hamiltonian (1),

$$H_{\mathrm{XXZ}} = 2J \operatorname{sh}(\eta) \sum_{j=1}^{L} \partial_\lambda (PR)_{j-1,j}(\lambda, 0)|_{\lambda=0} \tag{4}$$

(P is the permutation matrix, $\operatorname{ch}(\eta) = \Delta$ in (1)), but also a related auxiliary vertex model whose partition function in a certain 'Trotter limit' is equal to the partition function of the XXZ Hamiltonian. Details of this construction in a notation also suitable for our present purpose were reviewed in our paper [7]. Here we shall repeat only the most important formulae as far as they are needed to understand the notation below. We define the monodromy matrix of the auxiliary vertex model as

$$T_j(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}_j = R_{j\overline{N}}\left(\lambda, \frac{\beta}{N}\right) R^{t_1}_{\overline{N-1}j}\left(-\frac{\beta}{N}, \lambda\right) \cdots R_{j\overline{2}}\left(\lambda, \frac{\beta}{N}\right) R^{t_1}_{\overline{1}j}\left(-\frac{\beta}{N}, \lambda\right), \tag{5}$$

where t_1 means transposition with respect to the first space, and the parameter β is inversely proportional to the temperature T,

$$\beta = \frac{2J\operatorname{sh}(\eta)}{T}. \tag{6}$$

The monodromy matrix (5) acts in the tensor product of an auxiliary space j and N 'quantum spaces' $\overline{1}, \ldots, \overline{N}$. It generates a representation of the Yang–Baxter algebra with R-matrix (2). The corresponding transfer matrix

$$t(\lambda) = \operatorname{tr}_j T_j(\lambda), \tag{7}$$

called the quantum transfer matrix, defines a vertex model, whose partition function in the Trotter limit $N \to \infty$ is equal to the partition function $Z_L = \operatorname{tr} \exp(-H_{\mathrm{xxz}}/T)$ of the XXZ chain of length L,

$$Z_L = \lim_{N\to\infty} \operatorname{tr}_{\overline{1},\ldots,\overline{N}} (t(0))^L = \sum_{j=0}^{\infty} \Lambda_n^L(0). \tag{8}$$

Here $\Lambda_n(\lambda)$ denotes the nth eigenvalue of the quantum transfer matrix. Note that there is a unique real eigenvalue $\Lambda_0(\lambda)$ with largest modulus which dominates the partition function in the thermodynamic limit, when L goes to infinity. This single leading eigenvalue determines the bulk thermodynamics of the XXZ chain. We showed in [7] that the corresponding eigenvector determines the state of thermodynamic equilibrium completely. It fixes all finite temperature correlation functions (compare [23, 24]).

Due to the conservation of the z-component of the total spin

$$S^z = \frac{1}{2}\sum_{j=1}^{L}\sigma_j^z \tag{9}$$

thermodynamics and finite temperature correlation functions can still be treated within the quantum transfer matrix approach if the system is exposed to an external magnetic field h in z-direction [7]. The external field is properly taken into account by applying a twist to the monodromy matrix (5),

$$T(\lambda) \to T(\lambda)\begin{pmatrix} \mathrm{e}^{h/2T} & 0 \\ 0 & \mathrm{e}^{-h/2T}\end{pmatrix}. \tag{10}$$

3. Integral formula for density matrix elements

We shall use the notation

$$e_1^1 = \begin{pmatrix} 1 & 0 \\ 0 & 0\end{pmatrix}, \qquad e_1^2 = \begin{pmatrix} 0 & 1 \\ 0 & 0\end{pmatrix}, \qquad e_2^1 = \begin{pmatrix} 0 & 0 \\ 1 & 0\end{pmatrix}, \qquad e_2^2 = \begin{pmatrix} 0 & 0 \\ 0 & 1\end{pmatrix} \tag{11}$$

for the gl(2) standard basis. The canonical embedding of these matrices into the space of operators on the space of states $(\mathbb{C}^2)^{\otimes L}$ of the Hamiltonian (1) will be denoted by ${e_j}^\alpha_\beta, \alpha, \beta = 1, 2, j = 1, \ldots, L$. Then every operator $A_{1,\ldots,m}$ that acts on sites 1 to m of the spin chain can be expanded as

$$A_{1,\ldots,m} = A^{\beta_1\cdots\beta_m}_{\alpha_1\cdots\alpha_m}{e_1}^{\alpha_1}_{\beta_1}\cdots{e_m}^{\alpha_m}_{\beta_m}, \tag{12}$$

where implicit summation over the Greek indices is implied. The thermal average of such type of operator is

$$\langle A_{1,\ldots,m}\rangle_{T,h} = A^{\beta_1\cdots\beta_m}_{\alpha_1\cdots\alpha_m}\big\langle{e_1}^{\alpha_1}_{\beta_1}\cdots{e_m}^{\alpha_m}_{\beta_m}\big\rangle_{T,h}. \tag{13}$$

Thus, it is sufficient to calculate the expectation values $\big\langle{e_1}^{\alpha_1}_{\beta_1}\ldots{e_m}^{\alpha_m}_{\beta_m}\big\rangle_{T,h}$ which define the matrix elements of the density matrix of a chain segment of length m.

Following [7] we can calculate the general density matrix element as a limit of an appropriately defined inhomogeneous finite Trotter number approximant,

$$\big\langle{e_1}^{\alpha_1}_{\beta_1}\cdots{e_m}^{\alpha_m}_{\beta_m}\big\rangle_{T,h} = \lim_{N\to\infty}\lim_{\xi_1,\ldots,\xi_m\to 0}{D_N}^{\alpha_1\cdots\alpha_m}_{\beta_1\cdots\beta_m}(\xi_1,\ldots,\xi_m), \tag{14}$$

where

$${D_N}^{\alpha_1\cdots\alpha_m}_{\beta_1\cdots\beta_m}(\xi_1,\ldots,\xi_m) = \frac{\langle\{\lambda\}|T^{\alpha_1}_{\beta_1}(\xi_1)\cdots T^{\alpha_m}_{\beta_m}(\xi_m)|\{\lambda\}\rangle}{\langle\{\lambda\}|\prod_{j=1}^m t(\xi_j)|\{\lambda\}\rangle} \tag{15}$$

for $\alpha_j, \beta_k = 1, 2$, and $|\{\lambda\}\rangle = B(\lambda_1)\cdots B(\lambda_{N/2})|0\rangle$ is the eigenstate corresponding to the leading eigenvalue $\Lambda_0(\lambda)$ which is parametrized by a specific set of Bethe roots $\{\lambda\} = \{\lambda_j\}_{j=1}^{N/2}$. The complex inhomogeneity parameters ξ_j 'regularize' the expression in the numerator on the right-hand side of (15). Moreover, at least in the zero-temperature case, it turned out to be useful and interesting to study the dependence of D_N on these parameters [1, 4].

Table 1. Example for the definition of the sequences (α_j^+), (β_j^-), $(\widetilde{\alpha}_j^+)$ and $(\widetilde{\beta}_j^-)$. The pattern corresponds to the string $D(\xi_1)C(\xi_2)B(\xi_3)B(\xi_4)D(\xi_5)A(\xi_6)C(\xi_7)D(\xi_8)$ of monodromy matrix elements, $m = 8$, $|\alpha^+| = 3$, $|\beta^-| = 5$. The sequences (γ_j) and $(\gamma_j^\pm)$ are defined in section 4 where they are needed.

j	1	2	3	4	5	6	7	8
α_j	↓	↓	↑	↑	↓	↑	↓	↓
β_j	↓	↑	↓	↓	↓	↑	↑	↓
α_j^+	3	4	6					
β_j^-	1	3	4	5	8			
$\widetilde{\alpha}_j^+$	6	4	3					
$\widetilde{\beta}_j^-$				1	3	4	5	8
γ_j	1	3	3	4	4	5	6	8
γ_j^+	3	5	7					
γ_j^-	1	2	4	6	8			

We may identify values 1 of the indices with the symbol ↑, representing an up-spin, and values 2 with ↓, representing a down-spin. Then the upper and lower indices $(\alpha_n)_{n=1}^m$ and $(\beta_n)_{n=1}^m$ in e.g. (15) may be visualized as sequences of up- and down-spins. We shall denote the position n of the jth up-spin in the sequence $(\alpha_n)_{n=1}^m$ by α_j^+ and the number of up-spins in $(\alpha_n)_{n=1}^m$ by $|\alpha^+|$. Similarly we define β_j^- as the position of the jth down-spin in $(\beta_n)_{n=1}^m$ and denote the number of down-spins in $(\beta_n)_{n=1}^m$ by $|\beta^-|$. This yields two sequences $\left(\alpha_j^+\right)_{j=1}^{|\alpha^+|}$ and $(\beta_j^-)_{j=1}^{|\beta^-|}$ which we reorder and shift by the prescription $\widetilde{\alpha}_j^+ = \alpha^+_{|\alpha^+|-j+1}$, $j = 1, \ldots, |\alpha^+|$, and $\widetilde{\beta}_j^- = \beta^-_{j-|\alpha^+|}$, $j = |\alpha^+| + 1, \ldots, |\alpha^+| + |\beta^-|$. The definitions are illustrated with an example in table 1.

Due to the conservation of the total spin the matrix elements $D_N{}^{\alpha_1\cdots\alpha_m}_{\beta_1\cdots\beta_m}(\xi_1, \ldots, \xi_m)$ vanish if $|\alpha^+| + |\beta^-| \neq m$. They are non-trivial only if $|\alpha^+| + |\beta^-| = m$. For this case we suggest the integral representation

$$\begin{aligned} D_N{}^{\alpha_1\cdots\alpha_m}_{\beta_1\cdots\beta_m}(\xi_1, \ldots, \xi_m) = {} & \prod_{j=1}^{|\alpha^+|} \int_{\mathcal{C}} \frac{\mathrm{d}\omega_j}{2\pi \mathrm{i}(1 + \mathfrak{a}(\omega_j))} \prod_{k=1}^{\widetilde{\alpha}_j^+ - 1} \mathrm{sh}(\omega_j - \xi_k - \eta) \prod_{k=\widetilde{\alpha}_j^+ + 1}^{m} \mathrm{sh}(\omega_j - \xi_k) \\ & \times \prod_{j=|\alpha^+|+1}^{m} \int_{\mathcal{C}} \frac{\mathrm{d}\omega_j}{2\pi \mathrm{i}(1 + \overline{\mathfrak{a}}(\omega_j))} \prod_{k=1}^{\widetilde{\beta}_j^- - 1} \mathrm{sh}(\omega_j - \xi_k + \eta) \prod_{k=\widetilde{\beta}_j^- + 1}^{m} \mathrm{sh}(\omega_j - \xi_k) \\ & \times \frac{\det(-G(\omega_j, \xi_k))}{\prod_{1 \leqslant j < k \leqslant m} \mathrm{sh}(\xi_k - \xi_j)\mathrm{sh}(\omega_j - \omega_k - \eta)}. \end{aligned} \tag{16}$$

Equation (16) holds for any finite Trotter number N. The Trotter number enters the right-hand side of (16) implicitly through the functions $\mathfrak{a}(\omega)$, $\overline{\mathfrak{a}}(\omega) = 1/\mathfrak{a}(\omega)$ and $G(\omega, \xi)$. Performing the Trotter limit for D_N means to replace these functions by their respective Trotter limits. For brevity we show only the nonlinear integral equation that determines the Trotter limit of $\mathfrak{a}$,

$$\ln \mathfrak{a}(\lambda) = -\frac{h}{T} - \frac{2J\,\mathrm{sh}^2(\eta)}{T\,\mathrm{sh}(\lambda)\mathrm{sh}(\lambda + \eta)} - \int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi \mathrm{i}} \frac{\mathrm{sh}(2\eta) \ln(1 + \mathfrak{a}(\omega))}{\mathrm{sh}(\lambda - \omega + \eta)\mathrm{sh}(\lambda - \omega - \eta)}. \tag{17}$$

The corresponding finite Trotter number equation can be found in [7]. The function $G(\omega, \xi)$ which was introduced in [7] has to be calculated from the linear integral equation

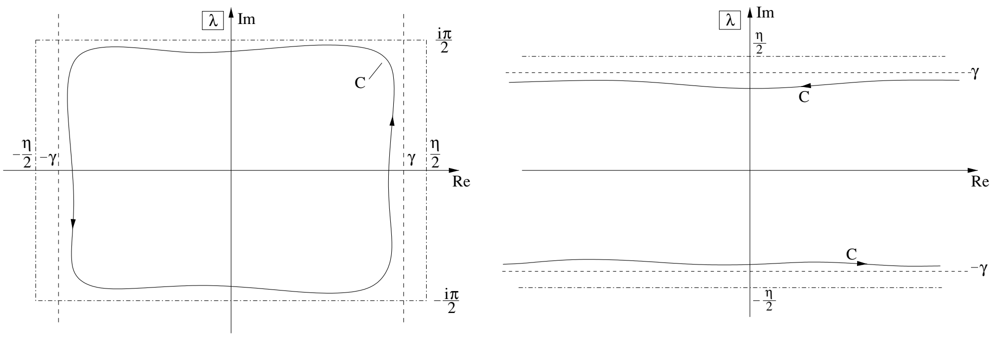

Figure 1. The canonical contour $\mathcal{C}$ in the off-critical regime $\Delta > 1$ (left panel) and in the critical regime $|\Delta| < 1$ (right panel). For $\Delta > 1$ the contour is a rectangle with sides at $\pm \mathrm{i}\frac{\pi}{2}$ and $\pm\gamma$, where γ is slightly smaller than $\frac{\eta}{2}$. For $|\Delta| < 1$ the contour surrounds the real axis at a distance $|\gamma|$ slightly less than $\frac{|\eta|}{2}$.

$$G(\lambda, \xi) = \frac{\mathrm{sh}(\eta)}{\mathrm{sh}(\xi - \lambda)\mathrm{sh}(\xi - \lambda + \eta)} + \int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}(1 + \mathfrak{a}(\omega))} \frac{\mathrm{sh}(2\eta)G(\omega, \xi)}{\mathrm{sh}(\lambda - \omega + \eta)\mathrm{sh}(\lambda - \omega - \eta)} \tag{18}$$

and generalizes the 'density function' $\rho(\lambda)$, which determines the ground-state energy and the zero-temperature magnetization, to finite temperatures and to the inhomogeneous case [7]. The canonical contour $\mathcal{C}$ in (16)–(18) depends on η and is shown in figure 1.

Our conjecture (16) is based on the following observations. (i) Equation (16) is true for $m = 1, 2$ which can easily be verified using the commutation relations comprised in the Yang–Baxter algebra and equations (98) and (104) of [7]. (ii) In two cases equation (16) reduces to the approximant to the emptiness formation probability, namely for $\alpha_j = \beta_j = 1$ for $j = 1, \ldots, m$ and $\alpha_j = \beta_j = 2$ for $j = 1, \ldots, m$. These two cases correspond to taking the limits $\varphi \to \pm\infty$ in our formulae for the generating function of the S^z–S^z correlation functions in [7]. One arrives at (16) by applying the result of appendix C of [12] (for more details see [6]). (iii) In the zero-temperature limit (16) reduces to the result of [14] which, in turns, generalizes the formulae [8, 9] of Jimbo *et al* to finite values of the external magnetic field. Some important intermediate steps of a proof of (16) in the general case are sketched in the next section.

Taking the Trotter limit and the homogeneous limit (for the latter compare [14]) in (16) we obtain an integral formula for the density matrix elements (14),

$$\begin{aligned} \left\langle e_1{}^{\alpha_1}_{\beta_1} \cdots e_m{}^{\alpha_m}_{\beta_m} \right\rangle_{T,h} = {} & \prod_{j=1}^{|\alpha^+|} \int_{\mathcal{C}} \frac{\mathrm{d}\omega_j}{2\pi\mathrm{i}(1 + \mathfrak{a}(\omega_j))} \mathrm{sh}^{\widetilde{\alpha}_j^+ - 1}(\omega_j - \eta)\mathrm{sh}^{m - \widetilde{\alpha}_j^+}(\omega_j) \\ & \times \prod_{j=|\alpha^+|+1}^{m} \int_{\mathcal{C}} \frac{\mathrm{d}\omega_j}{2\pi\mathrm{i}(1 + \overline{\mathfrak{a}}(\omega_j))} \mathrm{sh}^{\widetilde{\beta}_j^- - 1}(\omega_j + \eta)\mathrm{sh}^{m - \widetilde{\beta}_j^-}(\omega_j) \\ & \times \det\left[-\frac{\partial_\xi^{(k-1)} G(\omega_j, \xi)|_{\xi=0}}{(k-1)!} \right] \frac{1}{\prod_{1 \leqslant j < k \leqslant m} \mathrm{sh}(\omega_j - \omega_k - \eta)}. \end{aligned} \tag{19}$$

We should mention that the functions $1/(1 + \mathfrak{a}(\omega))$ and $1/(1 + \overline{\mathfrak{a}}(\omega))$, respectively, appear quite naturally here, since they generalize the Fermi functions for particles and holes to the interacting case.

4. Elements of a proof of the integral formula

In analogy with the example of the generating function of the S^z–S^z correlation functions treated in [7] we expect that a proof of the integral formula (16) for the general density matrix element can be achieved in three steps. Step 1 consists in calculating the action of a string of operators $T^{\alpha_1}_{\beta_1}(\xi_1)\cdots T^{\alpha_m}_{\beta_m}(\xi_m)$ on the left Bethe state $\langle\{\lambda\}| = \langle 0|C(\lambda_{N/2})\cdots C(\lambda_1)$. As is clear from the structure of the Yang–Baxter algebra, the result is a linear combination of vectors of the same form with some of the λ_j replaced with inhomogeneity parameters ξ_k. Step 2 is to calculate the scalar product of the vectors occurring in the sum of step 1 with the Bethe state $|\{\lambda\}\rangle$, to divide by the norm and by the product $\prod_{j=1}^m \Lambda_0(\xi_j)$ of transfer matrix eigenvalues, and to rewrite the resulting expression in a form that is suitable for taking the Trotter limit. This step is the same as in the derivation of the integral formula for the generating function of the S^z–S^z correlation function in [7]. Thus, we can use our former results.

Lemma 1 [7].

$$\frac{\langle\{\xi^+\}\cup\{\lambda^-\}|\{\lambda\}\rangle}{\langle\{\lambda\}|\{\lambda\}\rangle\prod_{j=1}^m\Lambda_0(\xi_j)} = \left[\prod_{j=1}^{|\lambda^-|}\prod_{k=1}^{|\lambda^+|} b\big(\lambda_j^-,\lambda_k^+\big)\right]\left[\prod_{j=1}^{|\xi^-|}\frac{1}{a(\xi_j^-)(1+\mathfrak{a}(\xi_j^-))}\prod_{k=1}^{|\lambda^-|} b(\lambda_k^-,\xi_j^-)\right]$$
$$\times\left[\prod_{j=1}^{|\lambda^+|}\frac{1}{a\big(\lambda_j^+\big)\mathfrak{a}'\big(\lambda_j^+\big)}\prod_{k=1}^{m} b\big(\lambda_j^+,\xi_k\big)\right]\left[\prod_{j,k=1}^{|\xi^+|}\frac{\mathrm{sh}\big(\lambda_j^+-\xi_k^++\eta\big)}{\mathrm{sh}\big(\lambda_j^+-\lambda_k^++\eta\big)}\right]$$
$$\times\left[\prod_{1\leqslant j<k\leqslant|\xi^+|}\frac{\mathrm{sh}\big(\lambda_j^+-\lambda_k^+\big)}{\mathrm{sh}\big(\xi_j^+-\xi_k^+\big)}\right]\det G\big(\lambda_j^+,\xi_k^+\big). \tag{20}$$

Here we divided the sets $\{\lambda\}$ and $\{\xi\}$ into disjoint subsets, $\{\lambda^\pm\}$ and $\{\xi^\pm\}$, and employed the notation $|X|$ for the number of elements in a set $\{X\}$. The function $a(\lambda)$ on the right-hand side is the vacuum eigenvalue of the monodromy matrix element $A(\lambda)$.

In step 3 we have to transform the sums obtained in steps 1 and 2 into integrals over the canonical contour $\mathcal{C}$. This involves the calculation of residua and the resummation of the many terms emerging in this procedure.

So far we could not complete step 3 in the general case, but only for examples of small m. Yet, we have obtained a complete and satisfactory result for step 1 that can be summarized in the following

Lemma 2. *Multiple action of monodromy matrix elements on a general state. Let $\lambda_1,\ldots,\lambda_{M+m}\in\mathbb{C}$ be mutually distinct. Then*

$$\langle 0|\left[\prod_{k=1}^{M}C(\lambda_k)\right]T^{\alpha_1}_{\beta_1}(\lambda_{M+1})\ldots T^{\alpha_m}_{\beta_m}(\lambda_{M+m})$$
$$=\sum_{\ell_1=1}^{M+\gamma_1}\sum_{\substack{\ell_2=1\\ \ell_2\neq\ell_1}}^{M+\gamma_2}\cdots\sum_{\substack{\ell_m=1\\ \ell_m\neq\ell_1,\ldots,\ell_{m-1}}}^{M+\gamma_m}\left[\prod_{j=1}^{|\alpha^+|} a\big(\lambda_{\ell_{\gamma_j^+}}\big)c\big(\lambda_{M+\alpha_j^+},\lambda_{\ell_{\gamma_j^+}}\big)\prod_{\substack{k=1\\ k\neq\ell_1,\ldots,\ell_{\gamma_j^+}}}^{M+\alpha_j^+}\frac{1}{b\big(\lambda_k,\lambda_{\ell_{\gamma_j^+}}\big)}\right]$$
$$\times\left[\prod_{j=1}^{m-|\alpha^+|} d\big(\lambda_{\ell_{\gamma_j^-}}\big)\times c\big(\lambda_{\ell_{\gamma_j^-}},\lambda_{M+\beta_j^-}\big)\prod_{\substack{k=1\\ k\neq\ell_1,\ldots,\ell_{\gamma_j^-}}}^{M+\beta_j^-}\frac{1}{b\big(\lambda_{\ell_{\gamma_j^-}},\lambda_k\big)}\right]\langle 0|\left[\prod_{\substack{k=1\\ k\neq\ell_1,\ldots,\ell_m}}^{M+m}C(\lambda_k)\right]. \tag{21}$$

Here $a(\lambda)$ and $d(\lambda)$ are the vacuum eigenvalues of $A(\lambda)$ and $D(\lambda)$, respectively. The sequences (α_j^+) and (β_k^-) were defined in section 3. We arrange all α_j^+ and β_k^- in non-decreasing order, in such a way that β_k^- appears left to α_j^+ if $\beta_k^- = \alpha_j^+$. This defines the sequence $(\gamma_n)_{n=1}^m$. The position of α_j^+ in this sequence is denoted by γ_j^+ and the position of β_k^- by γ_k^- (see table 1 for an example).

Lemma 2 can be proven by induction over m. Using the fact that $c(\lambda, \lambda) = 1$, the well-known [18] 'elementary' commutation relations for moving $A(\lambda)$, $B(\lambda)$ or $D(\lambda)$ through a product of Cs can be rewritten in the form

$$\langle 0| \left[\prod_{k=1}^{M} C(\lambda_k)\right] A(\lambda_{M+1}) = \sum_{\ell=1}^{M+1} a(\lambda_\ell) c(\lambda_{M+1}, \lambda_\ell) \left[\prod_{\substack{k=1\\k\neq\ell}}^{M+1} \frac{1}{b(\lambda_k, \lambda_\ell)}\right] \langle 0| \prod_{\substack{k=1\\k\neq\ell}}^{M+1} C(\lambda_k), \tag{22}$$

$$\langle 0| \left[\prod_{k=1}^{M} C(\lambda_k)\right] D(\lambda_{M+1}) = \sum_{\ell=1}^{M+1} d(\lambda_\ell) c(\lambda_\ell, \lambda_{M+1}) \left[\prod_{\substack{k=1\\k\neq\ell}}^{M+1} \frac{1}{b(\lambda_\ell, \lambda_k)}\right] \langle 0| \prod_{\substack{k=1\\k\neq\ell}}^{M+1} C(\lambda_k), \tag{23}$$

$$\begin{aligned}\langle 0| \left[\prod_{k=1}^{M} C(\lambda_k)\right] B(\lambda_{M+1}) = \sum_{\ell_1=1}^{M+1} \sum_{\substack{\ell_2=1\\ \ell_2\neq\ell_1}}^{M+1} d\big(\lambda_{\ell_1}\big) c\big(\lambda_{\ell_1}, \lambda_{M+1}\big) \left[\prod_{\substack{k=1\\k\neq\ell_1}}^{M+1} \frac{1}{b\big(\lambda_{\ell_1}, \lambda_k\big)}\right] \\ a\big(\lambda_{\ell_2}\big) c\big(\lambda_{M+1}, \lambda_{\ell_2}\big) \left[\prod_{\substack{k=1\\k\neq\ell_1,\ell_2}}^{M+1} \frac{1}{b\big(\lambda_k, \lambda_{\ell_2}\big)}\right] \langle 0| \prod_{\substack{k=1\\k\neq\ell_1,\ell_2}}^{M+1} C(\lambda_k).\end{aligned} \tag{24}$$

These formula prove (21) for $m = 1$. They can also be used in the induction step from $n \geqslant 1$ to $n + 1$.

In order to calculate the algebraic Bethe ansatz expression for the finite Trotter number approximant D_N, equation (15), we have to set $M = N/2$ in (21), then insert the solution $\{\lambda_j\}_{j=1}^{N/2}$ of the Bethe ansatz equation which belongs to the leading eigenvalue, then multiply by $\big|\{\lambda_j\}_{j=1}^{N/2}\big\rangle$ from the right and finally divide by $\langle\{\lambda\}|\{\lambda\}\rangle \prod_{j=1}^m \Lambda_0(\xi_j)$. The sums on the right-hand side of the resulting formula are naturally divided into a part from 1 to M over Bethe roots λ_j and a part from $M + 1$ to γ_j over inhomogeneities ξ_k. The sums over the Bethe roots (and only these) can be transformed into integrals over the canonical contour $\mathcal{C}$, since for any function $f(\omega)$ holomorphic on and inside $\mathcal{C}$ the identity

$$\int_{\mathcal{C}} \frac{\mathrm{d}\omega f(\omega)}{2\pi \mathrm{i}(1 + \mathfrak{a}(\omega))} = \sum_{j=1}^{N/2} \frac{f(\lambda_j)}{\mathfrak{a}'(\lambda_j)} = -\int_{\mathcal{C}} \frac{\mathrm{d}\omega f(\omega)}{2\pi \mathrm{i}(1 + \overline{\mathfrak{a}}(\omega))} \tag{25}$$

holds. If $f(\omega)$ is only meromorphic additional contributions appear due to the poles of $f(\omega)$. In any case it is clear that all sums over Bethe roots in the expression for D_N may be transformed into integrals over the contour $\mathcal{C}$ and that, after performing this transformation, a sum over multiple integrals will remain. These integrals will involve not more than m integrations, and the leading term involving precisely m integrations will be generated by the

m-fold sum from 1 to M over the Bethe roots,

$$\Theta = \sum_{\ell_1=1}^{M} \sum_{\substack{\ell_2=1 \\ \ell_2 \neq \ell_1}}^{M} \cdots \sum_{\substack{\ell_m=1 \\ \ell_m \neq \ell_1,\dots,\ell_{m-1}}}^{M} \left[\prod_{j=1}^{|\alpha^+|} a\big(\lambda_{\ell_{\gamma_j^+}}\big) c\big(\lambda_{M+\alpha_j^+}, \lambda_{\ell_{\gamma_j^+}}\big) \prod_{\substack{k=1 \\ k \neq \ell_1,\dots,\ell_{\gamma_j^+}}}^{M+\alpha_j^+} \frac{1}{b\big(\lambda_k, \lambda_{\ell_{\gamma_j^+}}\big)} \right]$$
$$\times \left[\prod_{j=1}^{m-|\alpha^+|} d\big(\lambda_{\ell_{\gamma_j^-}}\big) c\big(\lambda_{\ell_{\gamma_j^-}}, \lambda_{M+\beta_j^-}\big) \prod_{\substack{k=1 \\ k \neq \ell_1,\dots,\ell_{\gamma_j^-}}}^{M+\beta_j^-} \frac{1}{b\big(\lambda_{\ell_{\gamma_j^-}}, \lambda_k\big)} \right] \frac{\langle \{\xi\} \cup \{\lambda^-\} | \{\lambda\} \rangle}{\langle \{\lambda\} | \{\lambda\} \rangle \prod_{j=1}^{m} \Lambda_0(\xi_j)}, \tag{26}$$

where $\{\lambda^-\}$ is the complement of $\{\lambda^+\}$ in $\{\lambda\} = \{\lambda_j\}_{j=1}^{N/2}$, and $\{\lambda^+\} = \{\lambda_{\ell_1}, \dots, \lambda_{\ell_m}\}$. Inserting (20) into the right-hand side of (26) and using the Bethe ansatz equations (see [7]) we arrive at

$$\Theta = \sum_{\ell_1,\dots,\ell_m=1}^{M} \frac{\det\big(-G\big(\lambda_{\ell_j}, \xi_k\big)\big)}{\prod_{1 \leqslant j < k \leqslant m} \mathrm{sh}(\xi_k - \xi_j)\mathrm{sh}(\lambda_{\ell_k} - \lambda_{\ell_j} - \eta)} \left[\prod_{k=1}^{|\alpha^+|} \frac{1}{\mathfrak{a}'\big(\lambda_{\ell_k}\big)} \right]$$
$$\times \left[\prod_{j=1}^{|\alpha^+|} \prod_{k=1}^{\alpha_j^+ - 1} \mathrm{sh}\big(\lambda_{\ell_{|\alpha^+|-j+1}} - \xi_k - \eta\big) \prod_{k=\alpha_j^+ + 1}^{m} \mathrm{sh}\big(\lambda_{\ell_{|\alpha^+|-j+1}} - \xi_k\big) \right] \left[\prod_{k=|\alpha^+|+1}^{m} \frac{-1}{\mathfrak{a}'\big(\lambda_{\ell_k}\big)} \right]$$
$$\times \left[\prod_{j=1}^{m-|\alpha^+|} \prod_{k=1}^{\beta_j^- - 1} \mathrm{sh}\big(\lambda_{\ell_{|\alpha^+|+j}} - \xi_k + \eta\big) \prod_{k=\beta_j^- + 1}^{m} \mathrm{sh}\big(\lambda_{\ell_{|\alpha^+|+j}} - \xi_k\big) \right]. \tag{27}$$

Using (25) this expression turns into (16) plus a sum over terms involving less than m integrals. In other words, the right-hand side of (16) is the unique leading term as described above. Thus, our conjecture (16) means that the subleading terms mutually cancel each other. As mentioned above we verified this statement with a number of examples.

5. Discussion

We have presented new integral formulae for the density matrix of the XXZ chain (19) and for its inhomogeneous generalization (16). These formulae have been verified for the general matrix element for small m and for the special case of the emptiness formation probabilities for all m (note that $\big\langle e_1{}_1^1 \dots e_m{}_1^1 \big\rangle_{T,h}$ and $\big\langle e_1{}_2^2 \dots e_m{}_2^2 \big\rangle_{T,h}$ are different if $h \neq 0$). We also outlined two important steps of the proof of the general formula on which we are working now.

We think that our formulae have a great potential for applications in the calculation of finite temperature static correlation functions of the XXZ chain. We believe that the density matrix elements may efficiently be summed up [13]. We hope that for short segments the multiple integrals may be reduced to single integrals as e.g. in [10]. We have started to evaluate some of the integrals numerically. Last but not the least we are very curious if the analysis of the zero-temperature inhomogeneous case as developed in [1] carries over to finite temperatures.

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