Integral representations for correlation functions of the *XXZ* chain at finite temperature

2004 J. Phys. A: Math. Gen. 37 7625

(http://iopscience.iop.org/0305-4470/37/31/001)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **37** (2004) 7625–7651 PII: S0305-4470(04)80803-5

Integral representations for correlation functions of the *XXZ* chain at finite temperature

Frank Göhmann, Andreas Klümper and Alexander Seel

Fachbereich 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

Received 14 May 2004
Published 21 July 2004
Online at stacks.iop.org/JPhysA/37/7625
doi:10.1088/0305-4470/37/31/001

Abstract

We derive a novel multiple integral representation for a generating function of the σ^z–σ^z correlation functions of the spin-$\frac{1}{2}$ *XXZ* chain at finite temperature and finite, longitudinal magnetic field. Our work combines algebraic Bethe ansatz techniques for the calculation of matrix elements with the quantum transfer matrix approach to thermodynamics.

PACS numbers: 05.30.−d, 75.10.Pq

1. Introduction

The quantum transfer matrix [16, 17] is a means which makes it possible to calculate finite temperature properties of one-dimensional quantum spin systems. It becomes particularly efficient [7, 8] for the so-called integrable models which are related to representations of the Yang–Baxter algebra and are solvable by Bethe ansatz. Among these models the spin-$\frac{1}{2}$ *XXZ* chain (henceforth referred to as the *XXZ* chain) is one of the most thoroughly studied models (see, e.g., [2, 18, 12]). In contrast to many other integrable models, its spectral properties and thermodynamics are well understood. In addition, efficient formulae for norms [11], scalar products [15], and the multiple action of certain non-local operators [5] are available for the generalized model [11] defined by the *R*-matrix of the *XXZ* chain. These technical achievements led to the derivation of certain multiple integral representations for (static) two-point correlation functions and generating functions of two-point functions at zero temperature [5].

In this work we show how the results of [5] can be generalized to finite temperatures. We concentrate on the generating function of the σ^z–σ^z-correlation functions [3]. We use the quantum transfer matrix and the formalism of non-linear integral equations in order to express it as a multiple integral over the same auxiliary function that determines the free energy of the model. In the zero temperature limit we recover the result of [5]. An extension of our results to other finite temperature correlation functions of the *XXZ* chain is possible and will be published elsewhere.

After providing the necessary foundations for treating correlation functions at finite temperatures in section 2 we derive our main result in section 3, which is the integral formula (116) in theorem 1. As a special case of (116) we obtain an integral representation for the so-called emptiness formation probability [13] of the *XXZ* chain at finite temperature. In order to keep our presentation short, we formulate our results in the first instance only for the off-critical regime ($\Delta > 1$) of the model. Note, however, that our method applies for arbitrary values of the anisotropy parameter. In section 4 which is devoted to an outlook and to conclusions we indicate how our results have to be modified in the critical regime.

2. Foundations

2.1. Hamiltonian and R-matrix

The Hamiltonian of the L-site *XXZ* chain,

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

is defined on the L-fold tensor product $(\mathbb{C}^2)^{\otimes L}$ through the elementary operators $\sigma_j^\alpha, \alpha = x, y, z$, which act as Pauli matrices on the jth factor and trivially elsewhere. For $j = 0$ we set $\sigma_0^\alpha = \sigma_L^\alpha$, thereby specifying the boundary conditions to be periodic. $J > 0$ fixes the energy scale, and the real parameter Δ is the anisotropy parameter of the model.

The Hamiltonian (1) is closely related to a certain trigonometric solution

$$R(\lambda, \mu) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{\mathrm{sh}(\lambda-\mu)}{\mathrm{sh}(\lambda-\mu+\eta)} & \frac{\mathrm{sh}(\eta)}{\mathrm{sh}(\lambda-\mu+\eta)} & 0 \\ 0 & \frac{\mathrm{sh}(\eta)}{\mathrm{sh}(\lambda-\mu+\eta)} & \frac{\mathrm{sh}(\lambda-\mu)}{\mathrm{sh}(\lambda-\mu+\eta)} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{2}$$

of the Yang–Baxter equation which not only allows one to diagonalize the Hamiltonian by means of the algebraic Bethe ansatz, but will also enable us to associate a quantum transfer matrix with the model that will be our principal tool for calculating its finite temperature properties. We shall now briefly review the general theory.

For simplicity we shall restrict ourselves to fundamental models. These are models which are completely determined by a numerical $d^2 \times d^2$ matrix $R(\lambda, \mu) \in \mathrm{End}\left(\mathbb{C}^d \otimes \mathbb{C}^d\right)$ satisfying the Yang–Baxter equation[1]

$$R_{\alpha'\beta'}^{\alpha\beta}(\lambda, \mu) R_{\alpha''\gamma'}^{\alpha'\gamma}(\lambda, \nu) R_{\beta''\gamma''}^{\beta'\gamma'}(\mu, \nu) = R_{\beta'\gamma'}^{\beta\gamma}(\mu, \nu) R_{\alpha'\gamma''}^{\alpha\gamma'}(\lambda, \nu) R_{\alpha''\beta''}^{\alpha'\beta'}(\lambda, \mu). \tag{3}$$

This equation is nowadays not usually presented in components, but either graphically or in 'operator form' with respect to the gl(d) standard basis[2] canonically embedded into $\left(\mathbb{C}^d\right)^{\otimes L}$. In the latter case one defines

$$R_{jk}(\lambda, \mu) = R_{\beta\delta}^{\alpha\gamma}(\lambda, \mu) e_j{}_\alpha^\beta e_k{}_\gamma^\delta. \tag{4}$$

[1] Here and in the following we sum over doubly occurring Greek indices.

[2] The basis consists of all $d \times d$ matrices e_α^β having a single 1 at the intersection of the αth row with the βth column. Accordingly, the basis matrices multiply as $e_\alpha^\beta e_\gamma^\delta = \delta_\gamma^\beta e_\alpha^\delta$. The canonical embedding is defined by $e_j{}_\alpha^\beta = I_d^{\otimes(j-1)} \otimes e_\alpha^\beta \otimes I_d^{\otimes(L-j)}$ with I_d being the $d \times d$ unit matrix.

Then (3) is equivalent to

$$R_{12}(\lambda, \mu) R_{13}(\lambda, \nu) R_{23}(\mu, \nu) = R_{23}(\mu, \nu) R_{13}(\lambda, \nu) R_{12}(\lambda, \mu). \tag{5}$$

A Hamiltonian associated with the R-matrix $R(\lambda, \mu)$ is usually constructed as follows. First of all an L-matrix at site j with matrix elements

$$L_{j}{}^{\alpha}_{\beta}(\lambda, \mu) = R^{\alpha\gamma}_{\beta\delta}(\lambda, \mu) e_{j}{}^{\delta}_{\gamma} \tag{6}$$

is introduced. These matrix elements are operators in $(\mathrm{End}(\mathbb{C}^d))^{\otimes L}$. Multiplication of the Yang–Baxter equation (3) by $e_{j}{}^{\gamma''}_{\gamma}$ implies that

$$\check{R}(\lambda, \mu)(L_j(\lambda, \nu) \otimes L_j(\mu, \nu)) = (L_j(\mu, \nu) \otimes L_j(\lambda, \nu))\check{R}(\lambda, \mu), \tag{7}$$

where $\check{R}^{\alpha\gamma}_{\beta\delta} = R^{\gamma\alpha}_{\beta\delta}$. One says that $L_j(\lambda, \nu)$ is a representation of the Yang–Baxter algebra with R-matrix $R(\lambda, \mu)$. This representation is called the fundamental representation. Next, a monodromy matrix $T(\lambda)$ is introduced,

$$T(\lambda) = L_L(\lambda, \nu) \ldots L_1(\lambda, \nu). \tag{8}$$

Since $\left[L_{j+1}{}^{\alpha}_{\beta}(\lambda, \nu), L_{j}{}^{\gamma}_{\delta}(\lambda, \nu)\right] = 0$ it follows that

$$\check{R}(\lambda, \mu)(T(\lambda) \otimes T(\mu)) = (T(\mu) \otimes T(\lambda))\check{R}(\lambda, \mu). \tag{9}$$

This means that also $T(\lambda)$ is a representation of the Yang–Baxter algebra, a property which we use synonymously with integrability.

We shall assume that $R(\lambda, \mu)$ is regular in the sense that $R(0, 0) = P$ is the permutation matrix acting on $\mathbb{C}^d \otimes \mathbb{C}^d$. Then it follows that $L_{j}{}^{\alpha}_{\beta}(0, 0) = e_{j}{}^{\alpha}_{\beta}$ and further, setting $\nu = 0$ in (8), that the transfer matrix, defined as

$$t(\lambda) = \mathrm{Tr}(T(\lambda)), \tag{10}$$

has the expansion

$$t(\lambda) = \hat{U} \exp\{\lambda H + \mathcal{O}(\lambda^2)\} \tag{11}$$

around $\lambda = 0$. Here $\hat{U} = t(0)$ is the shift operator and

$$H = \hat{U}^{-1} t'(0) = \sum_{j=1}^{L} \partial_\lambda \check{R}_{j-1,j}(\lambda, 0)\Big|_{\lambda=0} \tag{12}$$

is the Hamiltonian associated with the fundamental representation (6) of the Yang–Baxter algebra. Note that periodic boundary conditions, $\check{R}_{01} = \check{R}_{L1}$, are implied in (12).

Employing the usual convention for tensor products we may interpret the matrix (2) as a linear operator in $\mathbb{C}^2 \otimes \mathbb{C}^2$. It is then easy to show that it satisfies the Yang–Baxter equation (3). Inserting (2) into the right-hand side of (12) we obtain

$$H = \frac{1}{2\,\mathrm{sh}(\eta)} \sum_{j=1}^{L} \left(\sigma^x_{j-1}\sigma^x_j + \sigma^y_{j-1}\sigma^y_j + \mathrm{ch}(\eta)\left(\sigma^z_{j-1}\sigma^z_j - 1\right)\right). \tag{13}$$

Thus,

$$H_{XXZ} = 2J\,\mathrm{sh}(\eta) H \tag{14}$$

if we identify $\Delta = \mathrm{ch}(\eta)$.

2.2. The Trotter–Suzuki formula

Consider the elementary formula

$$\lim_{N\to\infty}\left(1+\frac{X_N}{N}\right)^N = \mathrm{e}^X, \tag{15}$$

valid for any sequence $(X_N)_{N\in\mathbb{N}}$ of complex numbers converging to X. It still works [16] for a matrix (an operator) $X = -\beta H$. Hence, (11) and (15) imply that

$$\lim_{N\to\infty}\left(\hat{U}^{-1}t\left(-\frac{\beta}{N}\right)\right)^N = \lim_{N\to\infty}\left(1+\frac{1}{N}\left(-\beta H+\mathcal{O}\left(\frac{1}{N}\right)\right)\right)^N = \mathrm{e}^{-\beta H}. \tag{16}$$

This is a special form of the Trotter–Suzuki formula for the statistical operator $\mathrm{e}^{-H/T}$ if we choose β to be the inverse temperature, $\beta = 1/T$.

2.3. The quantum transfer matrix

We would like to use the Trotter–Suzuki formula (16) in a way that is compatible with the special structure of integrable models. In this context, it will turn out to be useful to introduce N auxiliary spaces denoted by indices $\bar{1},\ldots,\bar{N}$ and to work with R-operators rather than L-matrices.

We introduce two types of monodromy matrices: type one,

$$T_{\bar{j}}(\lambda) = R_{\bar{j}L}(\lambda,\mu)\ldots R_{\bar{j}1}(\lambda,\mu), \tag{17}$$

and type two,

$$\overline{T}_{\bar{j}}(\lambda) = R_{1\bar{j}}(\mu,\lambda)\ldots R_{L\bar{j}}(\mu,\lambda). \tag{18}$$

Remark. If R is unitary, $R_{12}(\lambda,\mu)R_{21}(\mu,\lambda) = \mathrm{id}$, then $\overline{T}_{\bar{j}}(\lambda) = T^{-1}_{\bar{j}}(\lambda)$.

By construction the trace of the monodromy matrix $T_{\bar{j}}(\lambda)$ with respect to the auxiliary space is the usual transfer matrix, $t(\lambda) = \mathrm{Tr}_{\bar{j}}(T_{\bar{j}}(\lambda))$. The structure of $\bar{t}(\lambda) = \mathrm{Tr}_{\bar{j}}(\overline{T}_{\bar{j}}(\lambda))$ can most easily be explored by means of the parity operator $\hat{P}$ which we define by its action on the canonical basis of local operators, $\hat{P}e_j{}^\alpha_\beta\hat{P} = e_{L-j+1}{}^\alpha_\beta$. Then

$$\overline{T}_{\bar{j}}(\lambda) = \hat{P}(PRP)_{\bar{j}L}(\mu,\lambda)\ldots(PRP)_{\bar{j}1}(\mu,\lambda)\hat{P}. \tag{19}$$

Here one has to be careful not to confuse the parity operator $\hat{P}$ with the permutation matrix P. In (19) we set $\mu = 0$, take the trace in space $\bar{j}$ and take into account that the parity operator acts only in quantum space. We infer with (11), (12) that

$$\begin{aligned}\bar{t}(\lambda) &= \hat{P}\hat{U}\exp\left\{\lambda\sum_{j=1}^{L}\partial_\lambda(PR\check{P})_{j-1j}(0,\lambda)\Big|_{\lambda=0}+\cdots\right\}\hat{P}\\ &= \exp\left\{\lambda\sum_{j=1}^{L}\partial_\lambda\check{R}_{j-1j}(0,\lambda)\Big|_{\lambda=0}+\mathcal{O}(\lambda^2)\right\}\hat{U}^{-1},\end{aligned} \tag{20}$$

where we used in the second equation that $(PRP)_{j-1j} = R_{jj-1}$ and $\hat{P}\hat{U}\hat{P} = \hat{U}^{-1}$.

In the following we shall assume that

$$\partial_\lambda\check{R}_{j-1j}(0,\lambda)|_{\lambda=0} = -\partial_\lambda\check{R}_{j-1,j}(\lambda,0)|_{\lambda=0}. \tag{21}$$

This is certainly true for R-matrices of difference form like (2) but also for other more general R-matrices like the R-matrix of the Hubbard model. Combining (11), (12), (20) and (21) we obtain

$$\rho_{N,L} := \left(\bar{t}\left(\frac{\beta}{N}\right) t\left(-\frac{\beta}{N}\right)\right)^{\frac{N}{2}} = \left(1 + \frac{2}{N}\left(-\beta H + \mathcal{O}\left(\frac{1}{N}\right)\right)\right)^{\frac{N}{2}}. \tag{22}$$

Using the second equation (16) we conclude that

$$\lim_{N\to\infty} \rho_{N,L} = \mathrm{e}^{-\beta H}. \tag{23}$$

The latter expression is very useful for integrable models. It leads us rather directly to the notion of the quantum transfer matrix, for we may write

$$\begin{aligned}
\rho_{N,L} &= \mathrm{Tr}_{\bar{1}\ldots\bar{N}}\left\{\overline{T}_{\bar{N}}\left(\frac{\beta}{N}\right) T_{\overline{N-1}}\left(-\frac{\beta}{N}\right)\ldots \overline{T}_{\bar{2}}\left(\frac{\beta}{N}\right) T_{\bar{1}}\left(-\frac{\beta}{N}\right)\right\} \\
&= \mathrm{Tr}_{\bar{1}\ldots\bar{N}}\left\{\overline{T}_{\bar{N}}\left(\frac{\beta}{N}\right) T^{t}_{\overline{N-1}}\left(-\frac{\beta}{N}\right)\ldots \overline{T}_{\bar{2}}\left(\frac{\beta}{N}\right) T^{t}_{\bar{1}}\left(-\frac{\beta}{N}\right)\right\} \\
&= \mathrm{Tr}_{\bar{1}\ldots\bar{N}}\left\{R_{1\bar{N}}\left(\mu,\frac{\beta}{N}\right) R_{2\bar{N}}\left(\mu,\frac{\beta}{N}\right)\ldots R_{L\bar{N}}\left(\mu,\frac{\beta}{N}\right)\right. \\
&\quad\times R^{t_1}_{\overline{N-1}1}\left(-\frac{\beta}{N},\mu\right) R^{t_1}_{\overline{N-1}2}\left(-\frac{\beta}{N},\mu\right)\ldots R^{t_1}_{\overline{N-1}L}\left(-\frac{\beta}{N},\mu\right) \\
&\qquad\qquad\qquad\cdots \\
&\quad\times R_{1\bar{2}}\left(\mu,\frac{\beta}{N}\right) R_{2\bar{2}}\left(\mu,\frac{\beta}{N}\right)\ldots R_{L\bar{2}}\left(\mu,\frac{\beta}{N}\right) \\
&\quad\times \left.\left. R^{t_1}_{\bar{1}1}\left(-\frac{\beta}{N},\mu\right) R^{t_1}_{\bar{1}2}\left(-\frac{\beta}{N},\mu\right)\ldots R^{t_1}_{\bar{1}L}\left(-\frac{\beta}{N},\mu\right)\right\}\right|_{\mu=0} \\
&= \mathrm{Tr}_{\bar{1}\ldots\bar{N}}\left\{R_{1\bar{N}}\left(\mu,\frac{\beta}{N}\right) R^{t_1}_{\overline{N-1}1}\left(-\frac{\beta}{N},\mu\right)\ldots R^{t_1}_{\bar{1}1}\left(-\frac{\beta}{N},\mu\right)\right. \\
&\qquad\qquad\qquad\cdots \\
&\quad\times \left.\left. R_{L\bar{N}}\left(\mu,\frac{\beta}{N}\right) R^{t_1}_{\overline{N-1}L}\left(-\frac{\beta}{N},\mu\right)\ldots R^{t_1}_{\bar{1}L}\left(-\frac{\beta}{N},\mu\right)\right\}\right|_{\mu=0} \\
&= \mathrm{Tr}_{\bar{1}\ldots\bar{N}}\left\{T^{QTM}_1(0)\ldots T^{QTM}_L(0)\right\}.
\end{aligned} \tag{24}$$

Here the transpose with respect to space 1 occurring in the third equation is defined by ${R^{t_1}}^{\alpha\gamma}_{\beta\delta} = R^{\beta\gamma}_{\alpha\delta}$. Note that we have reordered the product of R-matrices in the fourth equation and have introduced another monodromy matrix,

$$T^{\mathrm{QTM}}_j(\lambda) = R_{j\bar{N}}\left(\lambda,\frac{\beta}{N}\right) R^{t_1}_{\overline{N-1}j}\left(-\frac{\beta}{N},\lambda\right)\ldots R_{j\bar{2}}\left(\lambda,\frac{\beta}{N}\right) R^{t_1}_{\bar{1}j}\left(-\frac{\beta}{N},\lambda\right) \tag{25}$$

in the fifth equation. This monodromy matrix and the corresponding transfer matrix

$$t^{\mathrm{QTM}}(\lambda) = \mathrm{Tr}_j T^{\mathrm{QTM}}_j(\lambda), \tag{26}$$

which will be called the quantum transfer matrix, are our main tools for exploring the finite temperature properties of the *XXZ* chain below.

The quantum transfer matrix is useful mainly for two reasons. First, in the thermodynamic limit $L \to \infty$ a single leading eigenvalue of the quantum transfer matrix determines the free energy. Second, the spectrum of the quantum transfer matrix at finite Trotter number N can be calculated by means of the algebraic Bethe ansatz. Let us explain this in more detail.

Using (24) the partition function for a quantum chain of length L is calculated as

$$Z_L = \lim_{N\to\infty} \underbrace{\mathrm{Tr}_{1\ldots L}\rho_{N,L}}_{=:Z_{N,L}} = \lim_{N\to\infty} \mathrm{Tr}_{\bar{1}\ldots\bar{N}}(t^{\mathrm{QTM}}(0))^L = \sum_{n=1}^{\infty} \Lambda_n^L(0), \tag{27}$$

where the $\Lambda_n(0)$ are the eigenvalues of the quantum transfer matrix in the Trotter limit $N \to \infty$ at spectral parameter $\lambda = 0$. The free energy per lattice site in the thermodynamic limit is as follows,

$$f = -\lim_{L\to\infty}\lim_{N\to\infty} \frac{\ln(Z_{N,L})}{\beta L} = -\frac{\ln(\Lambda_0(0))}{\beta} \tag{28}$$

if $\Lambda_0(0)$ is the (finitely degenerate) leading eigenvalue of the quantum transfer matrix. For the remainder we shall accept the following:

(i) The limits $L \to \infty$ and $N \to \infty$ are interchangeable [16, 17].
(ii) The leading eigenvalue of the quantum transfer matrix is non-degenerate, real and positive and in the Trotter limit is separated from the next-to-leading eigenvalues by a gap.

The thermodynamics of the model under scrutiny is then determined by the leading eigenvalue $\Lambda_0(0)$ of the quantum transfer matrix in the Trotter limit $N \to \infty$.

We have seen that instead of calculating the infinitely many eigenvalues of the usual transfer matrix which determine the spectrum of the Hamiltonian it suffices to calculate a single eigenvalue of the quantum transfer matrix. Now we shall see that the quantum transfer matrix is a representation of the same Yang–Baxter algebra as the ordinary transfer matrix. Taking the transpose with respect to space 1 in (5) we obtain

$$R_{23}(\lambda,\mu)R_{12}^{t_1}(\nu,\lambda)R_{13}^{t_1}(\nu,\mu) = R_{13}^{t_1}(\nu,\mu)R_{12}^{t_1}(\nu,\lambda)R_{23}(\lambda,\mu). \tag{29}$$

Then, because of (5) and (29), the monodromy matrix (25) provides a representation of the Yang–Baxter algebra,

$$R_{jk}(\lambda,\mu)T_j^{\mathrm{QTM}}(\lambda)T_k^{\mathrm{QTM}}(\mu) = T_k^{\mathrm{QTM}}(\mu)T_j^{\mathrm{QTM}}(\lambda)R_{jk}(\lambda,\mu). \tag{30}$$

This means that the leading eigenvalue of the quantum transfer matrix may be obtained by algebraic Bethe ansatz (or possibly by one of the other powerful methods connected with the Yang–Baxter algebra as, e.g., the method of separation of variables [14]).

2.4. Correlation functions within the quantum transfer matrix approach

The quantum transfer matrix approach allows us to calculate, in principle, finite temperature correlation functions of local operators by means of the algebraic Bethe ansatz. Here we shall consider correlation functions of the form

$$\left\langle X_j^{(1)} \ldots X_k^{(k-j+1)}\right\rangle_T = \lim_{L\to\infty} \frac{\mathrm{Tr}_{1,\ldots,L}\, \mathrm{e}^{-\beta H} X_j^{(1)} \ldots X_k^{(k-j+1)}}{\mathrm{Tr}_{1,\ldots,L}\, \mathrm{e}^{-\beta H}}, \tag{31}$$

where $j, k \in \{1, \ldots, L\}$, $j \leqslant k$ and the $X_m^{(n)}$ are arbitrary local operators. Using (23) and (24) we rewrite (31) as

$$\begin{aligned}
&\left\langle X_j^{(1)} \ldots X_k^{(k-j+1)}\right\rangle_T \\
&\quad = \lim_{N,L\to\infty} \mathrm{Tr}_{\bar{1}\ldots\bar{N}}\mathrm{Tr}_{1\ldots L} T_1^{\mathrm{QTM}}(0)\ldots T_L^{\mathrm{QTM}}(0) X_j^{(1)}\ldots X_k^{(k-j+1)} \big/ Z_{N,L} \\
&\quad = \lim_{N,L\to\infty} \mathrm{Tr}_{\bar{1}\ldots\bar{N}}(t^{\mathrm{QTM}}(0))^{j-1}\mathrm{Tr}\{T^{\mathrm{QTM}}(0)X^{(1)}\}\ldots\mathrm{Tr}\{T^{\mathrm{QTM}}(0)X^{(k-j+1)}\} \\
&\qquad \times (t^{\mathrm{QTM}}(0))^{L-k}/Z_{N,L}
\end{aligned}$$

$$= \lim_{N,L\to\infty} \frac{\sum_{n=0}^{d^N-1} \Lambda_n^{L-k+j-1}(0)\langle\Psi_n|\mathrm{Tr}\{T^{\mathrm{QTM}}(0)X^{(1)}\}\dots\mathrm{Tr}\{T^{\mathrm{QTM}}(0)X^{(k-j+1)}\}|\Psi_n\rangle}{\sum_{n=0}^{d^N-1}\Lambda_n^L(0)}$$

$$= \lim_{N\to\infty} \Lambda_0^{j-k-1}(0)\langle\Psi_0|\mathrm{Tr}\{T^{\mathrm{QTM}}(0)X^{(1)}\}\dots\mathrm{Tr}\{T^{\mathrm{QTM}}(0)X^{(k-j+1)}\}|\Psi_0\rangle. \tag{32}$$

Here we assumed that the quantum transfer matrix is similar to a diagonal matrix[3] and has 'normalized' eigenvectors $|\Psi_n\rangle$. We see that a single normalized eigenvector $|\Psi_0\rangle$ and the corresponding eigenvalue $\Lambda_0(\lambda)$ of the quantum transfer matrix completely determine the finite temperature correlation functions of local operators.

Let us consider two examples related to the *XXZ* chain. In this case $d = 2$, and we can represent the monodromy matrix (25) as a 2×2 matrix

$$T^{\mathrm{QTM}}(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix} \tag{33}$$

in 'auxiliary space'.

Example. $X^{(1)} = \sigma^-$, $X^{(k-j+1)} = \sigma^+$, and all other $X^{(n)}$ are equal to the 2×2 unit matrix I_2. Then (32) turns into

$$\left\langle \sigma_j^- \sigma_k^+ \right\rangle_T = \lim_{N\to\infty} \Lambda_0^{j-k-1}(0)\langle\Psi_0|B(0)(A(0)+D(0))^{k-j-1}C(0)|\Psi_0\rangle. \tag{34}$$

Example. $X^{(1)} = X^{(2)} = \cdots = X^{(k-j+1)} = \mathrm{e}^{\varphi e_2^2} = \left(\begin{smallmatrix} 1 & 0 \\ 0 & \mathrm{e}^{\varphi}\end{smallmatrix}\right)$ and $j = 1, k = m$. In this case (32) turns into

$$\left\langle \exp\left\{\varphi \sum_{n=1}^{m} e_{n}{}_2^2\right\}\right\rangle_T = \lim_{N\to\infty} \Lambda_0^{-m}(0)\langle\Psi_0|(A(0)+\mathrm{e}^{\varphi}D(0))^m|\Psi_0\rangle. \tag{35}$$

This special correlation function [3] is a generating function of the σ^z–σ^z correlation functions which can be expressed as

$$\left\langle \sigma_1^z \sigma_m^z \right\rangle_T = \left(2D_m^2\partial_\varphi^2 - 4D_m\partial_\varphi + 1\right)\left\langle \exp\left\{\varphi\sum_{n=1}^{m} e_{n}{}_2^2\right\}\right\rangle_T\Bigg|_{\varphi=0}, \tag{36}$$

where D_m is the 'lattice derivative' defined on any complex sequence $(a_n)_{n\in\mathbb{N}}$ by $D_m a_m = a_m - a_{m-1}$. The function (35) generates a number of other interesting correlation functions that will be discussed below after we have derived an integral representation for (35).

The main goal of this work is to represent the generating function (35) as a multiple integral. The reason why we begin our study of finite temperature correlation functions with the generating function (35) and not with any two-point function like (34) is that (35) is slightly more simple than the other interesting correlation functions, because the individual factors in the product of operators on the right-hand side of (35) are closely related to the quantum transfer matrix.

The expectation value on the right-hand side of (35) cannot easily be calculated directly. Instead, we shall introduce an inhomogeneous version of it and shall perform the homogeneous limit only at the end of our calculation. We introduce a 'twisted quantum transfer matrix' of the *XXZ* chain as

$$t_\varphi(\lambda) = A(\lambda) + \mathrm{e}^{\varphi} D(\lambda). \tag{37}$$

[3] This is known for the *XXZ* chain, but not in the general case.

For brevity we have suppressed the label QTM here. It follows from the Yang–Baxter algebra (30) that the twisted quantum transfer matrices $t_\varphi(\lambda)$ for fixed φ form a commutative family,

$$[t_\varphi(\lambda), t_\varphi(\mu)] = 0. \tag{38}$$

For any set $\{\xi\} = \{\xi_j\}_{j=1}^m$, $\xi_j \in \mathbb{C}$, we define a function

$$\Phi_N(\varphi|\{\xi\}) = \langle\Psi_0| \left[\prod_{j=1}^m t_\varphi(\xi_j)\right] \left[\prod_{j=1}^m t_0^{-1}(\xi_j)\right] |\Psi_0\rangle \tag{39}$$

depending symmetrically (because of (38)) on the ξ_j. Then the generating function (35) can be calculated as

$$\left\langle \exp\left\{\varphi \sum_{n=1}^m e_{n\,2}^{\,2}\right\}\right\rangle_T = \lim_{N\to\infty} \lim_{\xi_1,\ldots,\xi_m\to 0} \Phi_N(\varphi|\{\xi\}). \tag{40}$$

Our strategy below will be to first calculate $\Phi_N(\varphi|\{\xi\})$ by means of the algebraic Bethe ansatz and then transform the resulting expression into a form that will allow us to perform the homogeneous limit and the Trotter limit on the right-hand side of (40).

2.5. Algebraic Bethe ansatz for the quantum transfer matrix

We shall now recall how to calculate spectrum and eigenvectors of the quantum transfer matrix by means of the algebraic Bethe ansatz. The result of an algebraic Bethe ansatz calculation is usually not explicit but expresses eigenvalues and eigenvectors in terms of the solutions of a set of Bethe ansatz equations. To actually solve the Bethe ansatz equations is another problem we deal with in the next section.

For the algebraic Bethe ansatz the form (9) of the Yang–Baxter algebra is more convenient than (30). Hence, we shall write the monodromy matrix (25) of the quantum transfer matrix as a 2×2 matrix. For this purpose, we first of all introduce two L-matrices L and $\tilde{L}$ setting

$$e_{a\,\alpha}^{\,\beta} L_{j\,\beta}^{\,\alpha}(\lambda,\mu) = R_{aj}(\lambda,\mu), \qquad e_{a\,\alpha}^{\,\beta} \tilde{L}_{j\,\beta}^{\,\alpha}(-\mu,\lambda) = R_{ja}^{t_1}(-\mu,\lambda). \tag{41}$$

Comparing these equations with the explicit expression (2) for the R-matrix of the *XXZ* chain we obtain the explicit forms of the two L-matrices,

$$L_j(\lambda,\mu) = \begin{pmatrix} e_{j\,1}^{\,1} + b(\lambda,\mu) e_{j\,2}^{\,2} & c(\lambda,\mu) e_{j\,2}^{\,1} \\ c(\lambda,\mu) e_{j\,1}^{\,2} & b(\lambda,\mu) e_{j\,1}^{\,1} + e_{j\,2}^{\,2} \end{pmatrix}, \tag{42a}$$

$$\tilde{L}_j(-\mu,\lambda) = \begin{pmatrix} e_{j\,1}^{\,1} + b(-\mu,\lambda) e_{j\,2}^{\,2} & c(-\mu,\lambda) e_{j\,1}^{\,2} \\ c(-\mu,\lambda) e_{j\,2}^{\,1} & b(-\mu,\lambda) e_{j\,1}^{\,1} + e_{j\,2}^{\,2} \end{pmatrix}, \tag{42b}$$

where we have employed the shorthand notation

$$b(\lambda,\mu) = \frac{\mathrm{sh}(\lambda-\mu)}{\mathrm{sh}(\lambda-\mu+\eta)}, \qquad c(\lambda,\mu) = \frac{\mathrm{sh}(\eta)}{\mathrm{sh}(\lambda-\mu+\eta)}. \tag{43}$$

When expressed in terms of the L-matrices (42) the monodromy matrix of the quantum transfer matrix becomes

$$T^{\mathrm{QTM}}(\lambda) = L_N\left(\lambda, \frac{\beta}{N}\right) \tilde{L}_{N-1}\left(-\frac{\beta}{N}, \lambda\right) \ldots \tilde{L}_1\left(-\frac{\beta}{N}, \lambda\right). \tag{44}$$

This is now a 2×2 matrix of the form (33) in 'auxiliary space' which satisfies the defining relations of the Yang–Baxter algebra of the form (9). Moreover, $T^{\mathrm{QTM}}(\lambda)$ acts as an upper triangular matrix on the vector

$$|0\rangle = (e_1 \otimes e_2)^{\otimes \frac{N}{2}} = \underbrace{\binom{1}{0} \otimes \binom{0}{1} \otimes \binom{1}{0} \otimes \cdots \binom{0}{1}}_{N \text{ factors}} \tag{45}$$

which is obvious from the form of the L-matrices (42). More precisely,

$$C(\lambda)|0\rangle = 0, \qquad A(\lambda)|0\rangle = a(\lambda)|0\rangle, \qquad D(\lambda)|0\rangle = d(\lambda)|0\rangle. \tag{46}$$

where

$$a(\lambda) = b\left(-\frac{\beta}{N}, \lambda\right)^{\frac{N}{2}} = \left(\frac{\mathrm{sh}\big(\lambda + \frac{\beta}{N}\big)}{\mathrm{sh}\big(\lambda + \frac{\beta}{N} - \eta\big)}\right)^{\frac{N}{2}}, \tag{47a}$$

$$d(\lambda) = b\left(\lambda, \frac{\beta}{N}\right)^{\frac{N}{2}} = \left(\frac{\mathrm{sh}\big(\lambda - \frac{\beta}{N}\big)}{\mathrm{sh}\big(\lambda - \frac{\beta}{N} + \eta\big)}\right)^{\frac{N}{2}}. \tag{47b}$$

The first equation (46) is sufficient for the algebraic Bethe ansatz to work. It can be performed for arbitrary pseudo-vacuum eigenvalues $a(\lambda)$ and $d(\lambda)$ of the diagonal elements of the monodromy matrix. These eigenvalues are often called 'the parameters of the algebraic Bethe ansatz'. Here they are given by (47). The parameters of the Bethe ansatz completely specify the solution which for the general case can, for instance, be read up in [12].

The vector

$$|\{\lambda\}\rangle = \big|\{\lambda_j\}_{j=1}^M\big\rangle = B(\lambda_1)\ldots B(\lambda_M)|0\rangle \tag{48}$$

is an eigenvector of the quantum transfer matrix $t_0(\lambda)$ if the rapidities (or Bethe roots) λ_j, $j = 1, \ldots, M$, satisfy the system

$$\frac{a(\lambda_j)}{d(\lambda_j)} = \prod_{\substack{k=1\\k\neq j}}^{M} \frac{\mathrm{sh}(\lambda_j - \lambda_k + \eta)}{\mathrm{sh}(\lambda_j - \lambda_k - \eta)} \tag{49}$$

of Bethe ansatz equations. The corresponding eigenvalue is

$$\Lambda(\lambda) = a(\lambda)\prod_{j=1}^{M}\frac{\mathrm{sh}(\lambda - \lambda_j - \eta)}{\mathrm{sh}(\lambda - \lambda_j)} + d(\lambda)\prod_{j=1}^{M}\frac{\mathrm{sh}(\lambda - \lambda_j + \eta)}{\mathrm{sh}(\lambda - \lambda_j)}. \tag{50}$$

Note that the 'creation operators' $B(\lambda_j)$ mutually commute. Therefore the eigenvector (48) is symmetric in the rapidities, hence our notation $|\{\lambda\}\rangle$.

2.6. Leading eigenvalue and auxiliary function

In order to calculate the approximant $\Phi_N(\varphi|\{\xi\})$ to the generating function (35) of the σ^z–σ^z correlation functions we need to know the specific solution $\{\lambda\}_{j=1}^M$ of the Bethe ansatz equations (49) that determines the leading eigenvalue $\Lambda_0(\lambda)$ and the corresponding eigenvector $|\Psi_0\rangle$. This solution cannot be obtained in a closed analytic form. Even worse, unlike in the case of the ordinary transfer matrix, the distribution of the Bethe roots cannot be approximated by a smooth 'density function' in the Trotter limit, since they accumulate in the vicinity of zero as N increases. A way out of these difficulties was proposed in [7, 8]. One associates an auxiliary function

$$\mathfrak{a}(\lambda) = \frac{d(\lambda)}{a(\lambda)}\prod_{k=1}^{N/2}\frac{\mathrm{sh}(\lambda - \lambda_k + \eta)}{\mathrm{sh}(\lambda - \lambda_k - \eta)} \tag{51}$$

with the solution $\{\lambda\} = \{\lambda_k\}_{k=1}^{\frac{N}{2}}$ of the Bethe ansatz equations that determines the leading eigenvalue of the quantum transfer matrix. It then turns out that the function $\mathfrak{a}(\lambda)$ is sufficiently well determined by the gross properties of $\{\lambda\}$. Knowing that the leading eigenvalue for fixed

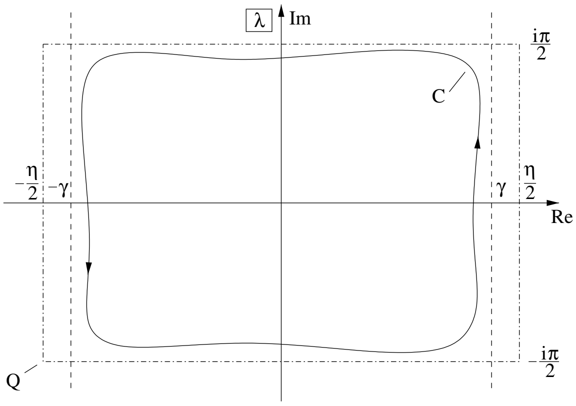

Figure 1. The canonical contour $\mathcal{C}$ for the off-critical regime $\Delta > 1$.

Trotter number N is determined by

(i) $M = N/2$ Bethe roots[4] which
(ii) are mutually distinct and
(iii) lie all on the imaginary axis

we can derive a non-linear integral equation which (alternatively) defines $\mathfrak{a}(\lambda)$. The details of the derivation have been described on several earlier occasions [9]. Here we only note that (i)–(iii) can be established 'perturbatively' in the high temperature limit and have been verified numerically for a wide range of Trotter numbers and temperatures. Conditions (i)–(iii) determine the analytical properties of the auxiliary function $\mathfrak{a}(\lambda)$:

(i) The auxiliary function $\mathfrak{a}$ is meromorphic and periodic with period $\mathrm{i}\pi$ in imaginary direction.
(ii) It has $3N/2$ poles (including multiplicities) in the fundamental domain $D = \{z \in \mathbb{C} | -\pi/2 < |\mathrm{Im}\, z| \leqslant \pi/2\}$: $N/2$ simple poles at $\lambda_j + \eta$, $j = 1, \ldots, N/2$; an $N/2$-fold pole at $\lambda = -\beta/N$; and an $N/2$-fold pole at $\lambda = \beta/N - \eta$.
(iii) The meromorphic function $1 + \mathfrak{a}$ has $3N/2$ zeros in D: $N/2$ simple zeros at the Bethe ansatz roots,

$$1 + \mathfrak{a}(\lambda_j) = 0, \tag{52}$$

clustering close to $\lambda = 0$ as $\beta \to 0$; $N/2$ zeros which are close to η as $\beta \to 0$; and $N/2$ zeros which accumulate at $-\eta$ for $\beta \to 0$. We assume for the latter two kinds of zeros that the modulus of their real part stays larger than $\eta/2$ for all finite temperatures.

Once the analytical properties of $\mathfrak{a}$ and $1 + \mathfrak{a}$ are established it is not difficult to derive the following integral equation for the auxiliary function,

$$\ln \mathfrak{a}(\lambda) = \ln \left[\frac{\mathrm{sh}\big(\lambda - \frac{\beta}{N}\big) \mathrm{sh}\big(\lambda + \frac{\beta}{N} + \eta\big)}{\mathrm{sh}\big(\lambda + \frac{\beta}{N}\big)\, \mathrm{sh}\big(\lambda - \frac{\beta}{N} + \eta\big)} \right]^{\frac{N}{2}} - \int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi \mathrm{i}} \frac{\mathrm{sh}(2\eta) \ln(1 + \mathfrak{a}(\omega))}{\mathrm{sh}(\lambda - \omega + \eta)\, \mathrm{sh}(\lambda - \omega - \eta)}, \tag{53}$$

where (for $\Delta > 1$) the contour $\mathcal{C}$ (see figure 1) is a rectangular contour with edges parallel to the real axis at $\pm \mathrm{i}\pi/2$ and to the imaginary axis at $\pm\gamma$ where $0 < \gamma < \eta/2$. Equation (53) is valid inside the rectangle Q defined by $|\mathrm{Re}\, \lambda| < \eta/2$ and $|\mathrm{Im}\, \lambda| < \pi/2$. This means that it defines the auxiliary function $\mathfrak{a}(\lambda)$ for all other λ in Q once it has been calculated on $\mathcal{C}$.

[4] This was already used in the definition (51) of $\mathfrak{a}(\lambda)$. For technical reasons we assume that $N/4 \in \mathbb{N}$.

In particular, one may calculate the zeros of $1 + \mathfrak{a}$ inside $\mathcal{C}$ which, by construction (see (52)), are those solutions of the Bethe ansatz equations that determine the leading eigenvalue and the corresponding eigenvector. We will, however, not use equation (53) in this way. It turns out that all quantities we are interested in, the free energy and the generating function of the σ^z–σ^z correlation functions in particular, can be expressed as integrals over the auxiliary function $\mathfrak{a}$ on the contour $\mathcal{C}$.

It is very important that the contour $\mathcal{C}$ of the integral on the right-hand side of (53) does not depend on N. The Trotter number N merely appears as a parameter in the inhomogeneity of the integral equation. Hence, the Trotter limit can be performed in (53). We obtain

$$\ln \mathfrak{a}(\lambda) = -\frac{2J\,\mathrm{sh}^2(\eta)}{T\,\mathrm{sh}(\lambda)\,\mathrm{sh}(\lambda+\eta)} - \int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{\mathrm{sh}(2\eta)\ln(1+\mathfrak{a}(\omega))}{\mathrm{sh}(\lambda-\omega+\eta)\,\mathrm{sh}(\lambda-\omega-\eta)}. \tag{54}$$

Here we already took into account the rescaling of the Hamiltonian (see (14) and (16)) and introduced the temperature T as

$$T = \frac{2J\,\mathrm{sh}(\eta)}{\beta}. \tag{55}$$

The auxiliary function $\mathfrak{a}$ encodes the information about the location of those Bethe roots that determine the leading eigenvalue of the quantum transfer matrix and the corresponding eigenvector. Using the results of sections 2.3 and 2.4 we conclude that $\mathfrak{a}$ thus encodes not only the complete information about the free energy but also all the 'thermodynamically relevant information' about the correlation functions of local operators.

2.7. *Including the magnetic field*

Before coming to the calculation of physical quantities in the next sections, we have to discuss the issue of how to include a (longitudinal) magnetic field into the formalism. For this purpose, we have to replace the statistical operator $\mathrm{e}^{-\beta H}$ by $\mathrm{e}^{-(\beta H - hS^z/T)}$, where h denotes the magnetic field and

$$S^z = \frac{1}{2}\sum_{j=1}^{L} \sigma_j^z \tag{56}$$

is the operator of the z-component of the total spin.

The reason why this is a rather simple task lies in the commutativity of the R-matrix (2) with the tensorial square of the diagonal matrix $\Theta = \mathrm{diag}(\mathrm{e}^{\theta}, \mathrm{e}^{-\theta})$,

$$[R(\lambda,\mu), \Theta \otimes \Theta] = 0. \tag{57}$$

Taking the derivative of this equation with respect to θ at $\theta = 0$ we obtain

$$[R(\lambda,\mu), \sigma^z \otimes I_2 + I_2 \otimes \sigma^z] = 0. \tag{58}$$

The latter equation implies that the ordinary transfer matrix and hence the Hamiltonian commute with S^z. On the other hand (57) is equivalent to

$$\check{R}(\lambda,\mu)(\Theta\otimes\Theta) = (\Theta\otimes\Theta)\check{R}(\lambda,\mu), \tag{59}$$

which means that Θ is a spectral parameter independent representation of the Yang–Baxter algebra with R-matrix (2). It follows that

$$\lim_{N\to\infty} \rho_{N,L}\,\mathrm{e}^{\frac{hS^z}{T}} = \mathrm{e}^{-(\beta H - hS^z/T)}, \tag{60}$$

while, on the other hand,

$$\rho_{N,L}\,\mathrm{e}^{\frac{hS^z}{T}} = \mathrm{Tr}_{\bar{1},\dots,\bar{N}}\, T_1^{\mathrm{QTM}}(0)\begin{pmatrix}\mathrm{e}^{h/2T} & 0\\ 0 & \mathrm{e}^{-h/2T}\end{pmatrix}_1 \cdots T_L^{\mathrm{QTM}}(0)\begin{pmatrix}\mathrm{e}^{h/2T} & 0\\ 0 & \mathrm{e}^{-h/2T}\end{pmatrix}_L, \tag{61}$$

where $T_j^{\mathrm{QTM}}(\lambda)$ is the monodromy matrix corresponding to the quantum transfer matrix as defined for zero magnetic field.

Thus, we can include a longitudinal magnetic field by simply replacing

$$T^{\mathrm{QTM}}(\lambda) \to T^{\mathrm{QTM}}(\lambda) \begin{pmatrix} \mathrm{e}^{h/2T} & 0 \\ 0 & \mathrm{e}^{-h/2T} \end{pmatrix} \tag{62}$$

in our former calculations. The important point here is that, because of (59), the redefined monodromy matrix is still a representation of the Yang–Baxter algebra with the same R-matrix (2). Therefore our former calculations go through without almost any modification. We simply replace $a(\lambda)$ by $a(\lambda)\,\mathrm{e}^{h/2T}$ and $d(\lambda)$ by $d(\lambda)\,\mathrm{e}^{-h/2T}$ in (49)–(51). The only point one then has to take care of is that the loci of the Bethe roots that describe the leading eigenvalue are now off the imaginary axis. As a consequence the parameter γ appearing in our definition of the path above has to be chosen large enough (but still between zero and $\eta/2$). Then the only modification of the integral equations (53) and (54) is the appearance of an extra term $-h/T$ on the right-hand side. For example, (54) turns into

$$\ln \mathfrak{a}(\lambda) = -\frac{h}{T} - \frac{2J\,\mathrm{sh}^2(\eta)}{T\,\mathrm{sh}(\lambda)\,\mathrm{sh}(\lambda+\eta)} - \int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{\mathrm{sh}(2\eta)\ln(1+\mathfrak{a}(\omega))}{\mathrm{sh}(\lambda-\omega+\eta)\,\mathrm{sh}(\lambda-\omega-\eta)}. \tag{63}$$

This is the non-linear integral equation for the auxiliary function $\mathfrak{a}$ of the *XXZ* chain exposed to a finite, longitudinal magnetic field h.

It is often useful (in particular when it comes to numerical calculations) to consider the auxiliary function $\mathfrak{a}$ together with its 'dual' $\overline{\mathfrak{a}} = 1/\mathfrak{a}$. As we can see from equation (52) the function $\overline{\mathfrak{a}}$ is equally useful in determining the Bethe roots, for $1 + \mathfrak{a}(\lambda) = 0$ is equivalent to $1 + \overline{\mathfrak{a}}(\lambda) = 0$. An integral equation for $\overline{\mathfrak{a}}$ can be directly obtained from (63). For this purpose, we choose λ and ω from inside the rectangle Q. Then $|\mathrm{Re}\,\lambda|, |\mathrm{Re}\,\omega| < \eta/2$ and hence $\lambda - \omega \pm \eta \neq 0$. Taking this into account we change the free variable in equation (63) from λ to ω, multiply it by $\mathrm{sh}(2\eta)/2\pi\mathrm{i}\,\mathrm{sh}(\lambda-\omega+\eta)\,\mathrm{sh}(\lambda-\omega-\eta)$ and integrate over $\mathcal{C}$. The resulting formula is

$$\int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{\mathrm{sh}(2\eta)\ln(\mathfrak{a}(\omega))}{\mathrm{sh}(\lambda-\omega+\eta)\,\mathrm{sh}(\lambda-\omega-\eta)} = -\frac{2J\,\mathrm{sh}(\eta)\,\mathrm{sh}(2\eta)}{T\,\mathrm{sh}(\lambda+\eta)\,\mathrm{sh}(\lambda-\eta)}. \tag{64}$$

We use it in (63) and obtain an integral equation for $\overline{\mathfrak{a}}$:

$$\ln \overline{\mathfrak{a}}(\lambda) = \frac{h}{T} - \frac{2J\,\mathrm{sh}^2(\eta)}{T\,\mathrm{sh}(\lambda)\,\mathrm{sh}(\lambda-\eta)} + \int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{\mathrm{sh}(2\eta)\ln(1+\overline{\mathfrak{a}}(\omega))}{\mathrm{sh}(\lambda-\omega+\eta)\,\mathrm{sh}(\lambda-\omega-\eta)}. \tag{65}$$

Comparing this with (63) we see that the formal difference consists in replacing h and η by $-h$ and $-\eta$.

2.8. Free energy and magnetization

Starting from expression (50) (properly modified such as to include the magnetic field) we can derive expressions that represent the free energy per lattice site f as integrals either over $\mathfrak{a}$ or $\overline{\mathfrak{a}}$ (for details see [9]),

$$f(h,T) = -\frac{h}{2} - T\int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{\mathrm{sh}(\eta)\ln(1+\mathfrak{a}(\omega))}{\mathrm{sh}(\omega)\,\mathrm{sh}(\omega+\eta)} = \frac{h}{2} + T\int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{\mathrm{sh}(\eta)\ln(1+\overline{\mathfrak{a}}(\omega))}{\mathrm{sh}(\omega)\,\mathrm{sh}(\omega-\eta)}. \tag{66}$$

From these equations the thermodynamic properties of the *XXZ* chain can be calculated. For example, the magnetization per unit length of the chain at finite magnetic field h and finite temperature T, defined as

$$m(h,T) = \lim_{L\to\infty} \frac{\langle S^z \rangle_{h,T}}{L} \tag{67}$$

can be calculated by means of the thermodynamic relation

$$m(h,T) = -\frac{\partial f(h,T)}{\partial h}. \tag{68}$$

Introducing the function

$$\sigma(\lambda) = -\frac{T\partial_h \mathfrak{a}(\lambda)}{\mathfrak{a}(\lambda)} = \frac{T\partial_h \overline{\mathfrak{a}}(\lambda)}{\overline{\mathfrak{a}}(\lambda)} \tag{69}$$

and taking the derivative of (66) with respect to the magnetic field, we obtain

$$m(h,T) = -\frac{1}{2} - \int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{\mathrm{sh}(\eta)}{\mathrm{sh}(\omega)\,\mathrm{sh}(\omega-\eta)} \frac{\sigma(\omega)}{1+\mathfrak{a}(\omega)}. \tag{70}$$

Instead of calculating the explicit h-dependence of the functions $\mathfrak{a}$ or $\overline{\mathfrak{a}}$ and from this the function σ, we may calculate it from the linear integral equation

$$\sigma(\lambda) = 1 + \int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{\mathrm{sh}(2\eta)}{\mathrm{sh}(\lambda-\omega+\eta)\,\mathrm{sh}(\lambda-\omega-\eta)} \frac{\sigma(\omega)}{1+\mathfrak{a}(\omega)} \tag{71}$$

obtained from (65) by taking the derivative with respect to h. Equation (71) is numerically better conditioned than (69) and therefore particularly useful if one is interested in numbers.

For later use, we derive another formula for the magnetization using an analogy with the dressed function formalism for the density functions at zero temperature. We define a function $G(\lambda)$ as the solution of the linear integral equation

$$G(\lambda) = \frac{\mathrm{sh}(\eta)}{\mathrm{sh}(\lambda)\,\mathrm{sh}(\lambda-\eta)} + \int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{\mathrm{sh}(2\eta)}{\mathrm{sh}(\lambda-\omega+\eta)\,\mathrm{sh}(\lambda-\omega-\eta)} \frac{G(\omega)}{1+\mathfrak{a}(\omega)}. \tag{72}$$

Then it is not difficult to show that

$$\int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{\mathrm{sh}(\eta)}{\mathrm{sh}(\omega)\,\mathrm{sh}(\omega-\eta)} \frac{\sigma(\omega)}{1+\mathfrak{a}(\omega)} = \int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{G(\omega)}{1+\mathfrak{a}(\omega)}, \tag{73}$$

and it follows from (70), (72) that

$$m(h,T) = -\frac{1}{2} - \int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{G(\omega)}{1+\mathfrak{a}(\omega)} = \frac{1}{2} + \int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{G(\omega)}{1+\overline{\mathfrak{a}}(\omega)}. \tag{74}$$

3. Results

3.1. Combinatorics

We shall now derive our main result which is an integral formula for the generating function (35) of the σ^z–σ^z correlation functions of the *XXZ* chain. The general strategy we are going to pursue is to first calculate the inhomogeneous, finite Trotter number approximant $\Phi_N(\varphi|\{\xi\})$, equation (39), and then transform it into a form such that the limits in (40) can be performed.

The Bethe ansatz eigenvectors (48) are not 'normalized'. Hence, $\Phi_N(\varphi|\{\xi\})$, when expressed through the Bethe ansatz eigenvectors takes the form

$$\Phi_N(\varphi|\{\xi\}) = \frac{\langle\{\lambda\}|\big[\prod_{j=1}^m t_\varphi(\xi_j)\big]\big[\prod_{j=1}^m t_0^{-1}(\xi_j)\big]|\{\lambda\}\rangle}{\langle\{\lambda\}|\{\lambda\}\rangle}, \tag{75}$$

where the λ_j in $\{\lambda\}$ are those that characterize the leading eigenvalue. The dual $\langle\{\lambda\}|$ to $|\{\lambda\}\rangle$ can be expressed through the action of the operators $C(\lambda)$ (see (33)) on the dual pseudo-vacuum $\langle 0|$ which is the transposed form of $|0\rangle$,

$$\langle\{\lambda\}| = \langle 0|C(\lambda_1)\ldots C(\lambda_{N/2}). \tag{76}$$

In order to evaluate the numerator in (75) we calculate in the first instance the left action of $\prod_{j=1}^m t_\varphi(\xi_j)$ on $\langle\{\lambda\}|$. In this task we can largely follow [5]. The basic idea is to use the commutation relations

$$C(\mu)A(\lambda) = f(\mu,\lambda)A(\lambda)C(\mu) - g(\mu,\lambda)A(\mu)C(\lambda), \tag{77a}$$

$$C(\mu)D(\lambda) = f(\lambda,\mu)D(\lambda)C(\mu) - g(\lambda,\mu)D(\mu)C(\lambda) \tag{77b}$$

contained in the defining relations (9) of the Yang–Baxter algebra in order to move the operators A and D (implicit in the expression t_φ) in

$$\langle 0|C(\lambda_1)\ldots C(\lambda_{N/2})t_\varphi(\xi_1)\ldots t_\varphi(\xi_m) \tag{78}$$

to the left and replace them with their pseudo-vacuum expectation values a and d (which are the same for right action on the pseudo-vacuum and left action on its dual (see (42))). Our notation employed in (77) is

$$f(\lambda,\mu) = \frac{\mathrm{sh}(\lambda-\mu+\eta)}{\mathrm{sh}(\lambda-\mu)}, \qquad g(\lambda,\mu) = \frac{\mathrm{sh}(\eta)}{\mathrm{sh}(\lambda-\mu)}. \tag{79}$$

Except for the commutation relations (77) one needs in the actual calculation the mutual commutativity of the families of operators $C(\lambda)$ and $t_\varphi(\lambda)$, respectively,

$$[C(\lambda), C(\mu)] = [t_\varphi(\lambda), t_\varphi(\mu)] = 0, \tag{80}$$

which also follows from (9).

When we apply (77) successively in (78) in order to move the operators A and D to the very left, then the number of operators C per term in a single application of (77) is conserved. Merely the arguments of the commuted operators are exchanged in every possible way. To state this more formally we need to introduce an appropriate notation for sets and partitions of sets.

We shall deal with finite sets of complex numbers such as $\{\lambda_j\}_{j=1}^M$. For such sets we already introduced the shorthand notation $\{\lambda\} = \{\lambda_j\}_{j=1}^M$. Similarly we shall write $\{\xi\} = \{\xi_j\}_{j=1}^M$ etc. The number of elements in these sets will be somewhat loosely denoted as $|\lambda|, |\xi|, \ldots$. We further need partitions of sets into disjoint subsets. By $p_2\{\lambda\}$ we shall denote the set of all ordered pairs $(\{\lambda^+\}, \{\lambda^-\})$ of subsets $\{\lambda^+\}, \{\lambda^-\} \subset \{\lambda\}$ which satisfy $\{\lambda^+\} \cup \{\lambda^-\} = \{\lambda\}$ and $\{\lambda^+\} \cap \{\lambda^-\} = \emptyset$. The elements of the subsets $\{\lambda^\pm\}$ will be denoted by $\lambda_j^\pm$, such that we can write $\{\lambda^\pm\} = \{\lambda_j^\pm\}_{j=1}^{|\lambda^\pm|}$ if we want to emphasize the number of elements in the subsets. Using our new notation we conclude with (77) and (80) that

$$\langle\{\lambda\}|\prod_{j=1}^{|\xi|} t_\varphi(\xi_j) = \sum_{\substack{(\{\lambda^+\},\{\lambda^-\})\in p_2\{\lambda\}\\ (\{\xi^+\},\{\xi^-\})\in p_2\{\xi\}\\ |\xi^+|+|\lambda^-|=N/2}} R(\{\xi^+\}|\{\xi^-\}|\{\lambda^+\}|\{\lambda^-\})\langle\{\xi^+\}\cup\{\lambda^-\}| \tag{81}$$

with numerical coefficients R depending on the sets $\{\xi^\pm\}$, $\{\lambda^\pm\}$. These coefficients can be calculated in the general situation of arbitrary vacuum expectation values a, d of the diagonal elements of the monodromy matrix and for arbitrary sets of mutually distinct complex numbers $\{\xi\}$, $\{\lambda\}$, where the λ_j do not necessarily satisfy the Bethe ansatz equations.

Lemma 1 ([5]). *The coefficients* $R(\{\xi^+\}|\{\xi^-\}|\{\lambda^+\}|\{\lambda^-\})$ *in (81) are given by the formula*

$$R(\{\xi^+\}|\{\xi^-\}|\{\lambda^+\}|\{\lambda^-\}) = S(\{\xi^+\}|\{\lambda^+\}|\{\lambda^-\})\prod_{j=1}^{|\xi^-|}\left\{a(\xi_j^-)\left[\prod_{k=1}^{|\xi^+|} f\left(\xi_k^+,\xi_j^-\right)\right]\left[\prod_{l=1}^{|\lambda^-|} f(\lambda_l^-,\xi_j^-)\right]\right.$$
$$\left. + \mathrm{e}^\varphi d(\xi_j^-)\left[\prod_{k=1}^{|\xi^+|} f\left(\xi_j^-,\xi_k^+\right)\right]\left[\prod_{l=1}^{|\lambda^-|} f(\xi_j^-,\lambda_l^-)\right]\right\}, \tag{82}$$

where the so-called highest coefficient $S(\{\xi^+\}|\{\lambda^+\}|\{\lambda^-\})$ *can be expressed as the ratio of two determinants,*

$$S(\{\xi^+\}|\{\lambda^+\}|\{\lambda^-\}) = \frac{\det \widehat{M}\left(\lambda_j^+, \xi_k^+\right)}{\det V\left(\lambda_j^+, \xi_k^+\right)} \tag{83}$$

with

$$V\left(\lambda_j^+, \xi_k^+\right) = \frac{1}{\operatorname{sh}\left(\xi_k^+ - \lambda_j^+\right)}, \tag{84}$$

$$\begin{aligned}\widehat{M}\left(\lambda_j^+, \xi_k^+\right) = {} & a\left(\lambda_j^+\right) t\left(\xi_k^+, \lambda_j^+\right) \left[\prod_{l=1}^{|\xi^+|} f\left(\xi_l^+, \lambda_j^+\right)\right] \left[\prod_{m=1}^{|\lambda^-|} f\left(\lambda_m^-, \lambda_j^+\right)\right] \\ & - \mathrm{e}^{\varphi} d\left(\lambda_j^+\right) t\left(\lambda_j^+, \xi_k^+\right) \left[\prod_{l=1}^{|\xi^+|} f\left(\lambda_j^+, \xi_l^+\right)\right] \left[\prod_{m=1}^{|\lambda^-|} f\left(\lambda_j^+, \lambda_m^-\right)\right],\end{aligned} \tag{85}$$

$$t(\lambda, \xi) = \frac{\operatorname{sh}(\eta)}{\operatorname{sh}(\lambda - \xi) \operatorname{sh}(\lambda - \xi + \eta)}. \tag{86}$$

We may now insert (81) into (75) and use the fact, that the vector $|\{\lambda\}\rangle$ in (75) is the eigenvector of the quantum transfer matrix that belongs to the leading eigenvalue

$$\Lambda_0(\lambda) = a(\lambda) \prod_{j=1}^{N/2} f(\lambda_j, \lambda) + d(\lambda) \prod_{j=1}^{N/2} f(\lambda, \lambda_j) \tag{87}$$

(see (50)). We obtain

$$\Phi_N(\varphi|\{\xi\}) = \sum_{\substack{(\{\lambda^+\},\{\lambda^-\}) \in p_2\{\lambda\} \\ (\{\xi^+\},\{\xi^-\}) \in p_2\{\xi\} \\ |\xi^+| + |\lambda^-| = N/2}} \frac{R(\{\xi^+\}|\{\xi^-\}|\{\lambda^+\}|\{\lambda^-\})\langle\{\xi^+\} \cup \{\lambda^-\}|\{\lambda\}\rangle}{\left[\prod_{j=1}^{|\xi|} \Lambda_0(\xi_j)\right] \langle\{\lambda\}|\{\lambda\}\rangle}, \tag{88}$$

and only the ratio $\langle\{\xi^+\} \cup \{\lambda^-\}|\{\lambda\}\rangle / \langle\{\lambda\}|\{\lambda\}\rangle$ remains to be calculated. But here another combinatorial result for the *XXZ* chain applies.

Lemma 2 ([15])**.** *Let* $\{\lambda_j\}_{j=1}^M$ *be a solution of the Bethe ansatz equations (49) and* $\{\mu_k\}_{k=1}^M$ *any set of distinct complex numbers. Then*

$$\begin{aligned}&\langle 0|C(\mu_1) \ldots C(\mu_M) B(\lambda_1) \ldots B(\lambda_M)|0\rangle \\ &\quad = \frac{\left[\prod_{j=1}^M d(\lambda_j) a(\mu_j)\right] \prod_{j,k=1}^M \operatorname{sh}(\lambda_j - \mu_k + \eta)}{\prod_{1 \leqslant j < k \leqslant M} \operatorname{sh}(\lambda_j - \lambda_k) \operatorname{sh}(\mu_k - \mu_j)} \det \widehat{N}(\lambda_j, \mu_k),\end{aligned} \tag{89}$$

where

$$\widehat{N}(\lambda_j, \mu_k) = t(\lambda_j, \mu_k) - t(\mu_k, \lambda_j) \frac{d(\mu_k)}{a(\mu_k)} \prod_{l=1}^M \frac{f(\mu_k, \lambda_l)}{f(\lambda_l, \mu_k)}. \tag{90}$$

In order to apply lemma 2 to our task of calculating $\langle\{\xi^+\} \cup \{\lambda^-\}|\{\lambda\}\rangle / \langle\{\lambda\}|\{\lambda\}\rangle$ we first insert the set of Bethe roots that characterize the leading eigenvalue of the quantum transfer matrix into (89), (90). Then $M = N/2$, and the right-hand side of (90) can be expressed in terms of the auxiliary function (51),

$$\widehat{N}(\lambda_j, \mu_k) = t(\lambda_j, \mu_k) - t(\mu_k, \lambda_j)\mathfrak{a}(\mu_k). \tag{91}$$

Taking account of the Bethe ansatz equations $\mathfrak{a}(\lambda_k) = -1$ it is easy to study the limit $\mu_k \to \lambda_k$ in (89): the pre-factor is regular in this limit. Concerning the matrix $\widehat{N}$ only the kth column is affected,

$$\lim_{\mu_k \to \lambda_k} \widehat{N}(\lambda_j, \mu_k) = \delta^j_k \frac{\mathfrak{a}'(\lambda_k)}{\mathfrak{a}(\lambda_k)} + \frac{\mathrm{sh}(2\eta)}{\mathrm{sh}(\lambda_j - \lambda_k + \eta)\,\mathrm{sh}(\lambda_j - \lambda_k - \eta)}. \tag{92}$$

Adopting for a while the notation

$$\begin{aligned} \tilde{\lambda}_j &= \begin{cases} \lambda^+_j & \text{for} \quad j = 1, \ldots, |\xi^+| \\ \lambda^-_{j-|\xi^+|} & \text{for} \quad j = |\xi^+| + 1, \ldots, N/2, \end{cases} \\ \tilde{\xi}_j &= \xi^+_j \qquad\qquad \text{for} \quad j = 1, \ldots, |\xi^+| = n, \end{aligned} \tag{93}$$

we infer from (89)–(92) that

$$\begin{aligned} \frac{\langle \{\xi^+\} \cup \{\lambda^-\} | \{\lambda\} \rangle}{\langle \{\lambda\} | \{\lambda\} \rangle} &= \left[\prod_{j=1}^{n} \frac{a(\tilde{\xi}_j)}{a(\tilde{\lambda}_j)} \right] \left[\prod_{j=n+1}^{N/2} \prod_{k=1}^{n} \frac{f(\tilde{\lambda}_j, \tilde{\xi}_k)}{f(\tilde{\lambda}_j, \tilde{\lambda}_k)} \right] \\ &\quad \times \left[\prod_{j,k=1}^{n} \frac{\mathrm{sh}(\tilde{\lambda}_j - \tilde{\xi}_k + \eta)}{\mathrm{sh}(\tilde{\lambda}_j - \tilde{\lambda}_k + \eta)} \right] \left[\prod_{1 \leqslant j < k \leqslant n} \frac{\mathrm{sh}(\tilde{\lambda}_j - \tilde{\lambda}_k)}{\mathrm{sh}(\tilde{\xi}_j - \tilde{\xi}_k)} \right] \frac{\det N_n}{\det N_0}, \end{aligned} \tag{94}$$

where

$$N_n{}^j_k = \begin{cases} t(\tilde{\lambda}_j, \tilde{\xi}_k) - t(\tilde{\xi}_k, \tilde{\lambda}_j)\mathfrak{a}(\tilde{\xi}_k) & k = 1, \ldots, n \\ \delta^j_k \dfrac{\mathfrak{a}'(\tilde{\lambda}_k)}{\mathfrak{a}(\tilde{\lambda}_k)} + \dfrac{\mathrm{sh}(2\eta)}{\mathrm{sh}(\tilde{\lambda}_j - \tilde{\lambda}_k + \eta)\,\mathrm{sh}(\tilde{\lambda}_j - \tilde{\lambda}_k - \eta)} & k = n+1, \ldots, N/2. \end{cases} \tag{95}$$

The observation that the columns of N_n and N_0 are identical for $k > n$ allows one to simplify the ratio of the two determinants on the right-hand side of (94). In the appendix we prove the following:

Lemma 3. *The ratio of the two determinants on the right-hand side of (94) is proportional to the determinant of an $n \times n$ matrix,*

$$\frac{\det N_n}{\det N_0} = \left[\prod_{l=1}^{n} \frac{1 + \mathfrak{a}\big(\xi^+_l\big)}{\mathfrak{a}'\big(\lambda^+_l\big)} \right] \det G\big(\lambda^+_j, \xi^+_k\big), \tag{96}$$

where the function $G(\lambda, \xi)$ is the solution of the linear integral equation

$$G(\lambda, \xi) = t(\xi, \lambda) + \int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{\mathrm{sh}(2\eta)}{\mathrm{sh}(\lambda - \omega + \eta)\,\mathrm{sh}(\lambda - \omega - \eta)} \frac{G(\omega, \xi)}{1 + \mathfrak{a}(\omega)} \tag{97}$$

to be solved on the same canonical contour $\mathcal{C}$ as the non-linear integral equation for the auxiliary function $\mathfrak{a}$.

Note that $G(\lambda, \xi)$ is an inhomogeneous generalization of the 'finite temperature density function' $G(\lambda)$, equation (72), that determines the magnetization (74).

Using the lemma in (94) and switching back to our original notation we obtain the following result:

$$\frac{\langle\{\xi^+\}\cup\{\lambda^-\}|\{\lambda\}\rangle}{\langle\{\lambda\}|\{\lambda\}\rangle} = \left[\prod_{j=1}^{|\xi^+|}\frac{a(\xi_j^+)\left(1+\mathfrak{a}(\xi_j^+)\right)}{a(\lambda_j^+)\mathfrak{a}'(\lambda_j^+)}\right]\left[\prod_{j=1}^{|\lambda^-|}\prod_{k=1}^{|\xi^+|}\frac{f(\lambda_j^-,\xi_k^+)}{f(\lambda_j^-,\lambda_k^+)}\right]$$
$$\times\left[\prod_{j,k=1}^{|\xi^+|}\frac{\mathrm{sh}(\lambda_j^+-\xi_k^++\eta)}{\mathrm{sh}(\lambda_j^+-\lambda_k^++\eta)}\right]\left[\prod_{1\leqslant j<k\leqslant|\xi^+|}\frac{\mathrm{sh}(\lambda_j^+-\lambda_k^+)}{\mathrm{sh}(\xi_j^+-\xi_k^+)}\right]\det G(\lambda_j^+,\xi_k^+). \tag{98}$$

Finally, we use lemma 1 and equations (87), (98) in (88) and remove the explicit dependence on the λ_j^- from the resulting expression. The latter is possible by proper use of the auxiliary function $\mathfrak{a}$ and the Bethe ansatz equations (49). The calculation is elementary but slightly tedious. We obtain

Lemma 4. *The finite Trotter number approximant $\Phi_N(\varphi|\{\xi\})$, equation (75), has the following representation as a sum over partitions of the Bethe roots $\{\lambda\}$, which characterize the leading eigenvalue, and of the inhomogeneity parameters $\{\xi\}$,*

$$\Phi_N(\varphi|\{\xi\}) = \sum_{\substack{(\{\lambda^+\},\{\lambda^-\})\in p_2\{\lambda\}\\(\{\xi^+\},\{\xi^-\})\in p_2\{\xi\}\\|\xi^+|+|\lambda^-|=N/2}}\frac{Y_{|\xi^+|}(\{\lambda^+\}|\{\xi^+\})Z_{|\xi^+|}(\{\lambda^+\}|\{\xi^+\}|\{\xi^-\})}{\left[\prod_{j=1}^{|\xi^+|}\mathfrak{a}'(\lambda_j^+)\right]\left[\prod_{j=1}^{|\xi^-|}\left(1+\mathfrak{a}(\xi_j^-)\right)\right]}, \tag{99}$$

where the two functions $Y_n(\{\lambda^+\}|\{\xi^+\})$ and $Z_n(\{\lambda^+\}|\{\xi^+\}|\{\xi^-\})$ are defined as follows,

$$Y_n(\{\lambda^+\}|\{\xi^+\}) = \left[\prod_{j=1}^{n}\frac{\overline{\mathfrak{b}}(\lambda_j^+)}{\overline{\mathfrak{b}}'(\xi_j^+)}\right]\left[\prod_{j,k=1}^{n}\frac{\mathrm{sh}(\lambda_j^+-\xi_k^++\eta)\mathrm{sh}(\lambda_j^+-\xi_k^+-\eta)}{\mathrm{sh}(\xi_j^+-\xi_k^++\eta)\mathrm{sh}(\lambda_j^+-\lambda_k^+-\eta)}\right]$$
$$\times\widetilde{M}(\lambda_j^+,\xi_k^+)\det G(\lambda_j^+,\xi_k^+) \tag{100}$$

with

$$\overline{\mathfrak{b}}(\lambda) = \prod_{k=1}^{m}\frac{1}{f(\lambda,\xi_k)}, \tag{101}$$

$$\widetilde{M}(\lambda_j^+,\xi_k^+) = t(\xi_k^+,\lambda_j^+) + t(\lambda_j^+,\xi_k^+)\,\mathrm{e}^{\varphi}\prod_{l=1}^{n}\frac{\mathrm{sh}(\lambda_j^+-\lambda_l^+-\eta)\mathrm{sh}(\lambda_j^+-\xi_l^++\eta)}{\mathrm{sh}(\lambda_j^+-\lambda_l^++\eta)\mathrm{sh}(\lambda_j^+-\xi_l^+-\eta)}, \tag{102}$$

and $G(\lambda,\xi)$ is the solution of the linear integral equation (97).

$$Z_n(\{\lambda^+\}|\{\xi^+\}|\{\xi^-\}) = \prod_{j=1}^{m-n}\left[1+\mathrm{e}^{\varphi}\mathfrak{a}(\xi_j^-)\prod_{k=1}^{n}\frac{f(\xi_j^-,\xi_k^+)f(\lambda_k^+,\xi_j^-)}{f(\xi_k^+,\xi_j^-)f(\xi_j^-,\lambda_k^+)}\right]. \tag{103}$$

3.2. From sums to integrals

In the final step of our calculation, we would now like to express the sums over partitions in (99) as multiple integral over certain canonical paths. We shall apply a similar rationale as in [5, 6].

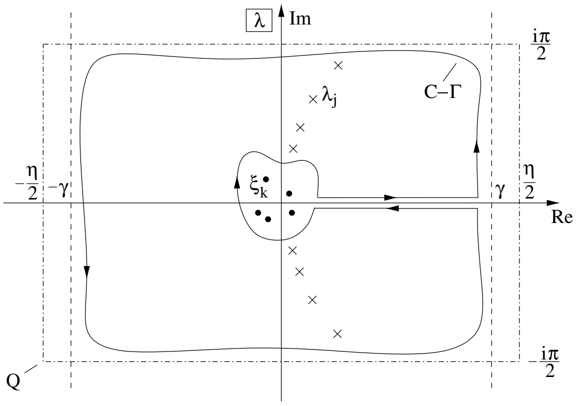

Figure 2. The path $\mathcal{C} - \Gamma$.

Consider a function $f(\omega_1, \dots, \omega_n) : \mathbb{C}^n \to \mathbb{C}$, symmetric in its arguments, equal to zero if any two of its arguments agree, and analytic on and inside the simple n-fold contour $\mathcal{C}^n$. The function $1 + \mathfrak{a}(\omega)$ is meromorphic inside the rectangle Q (see section 2.6), where its only zeros are the simple zeros located at those Bethe roots which characterize the leading eigenvalue of the quantum transfer matrix. Hence, the only poles of the meromorphic function $1/(1 + \mathfrak{a}(\omega))$ inside $\mathcal{C}$ are simple poles at the Bethe roots with residues

$$\operatorname{res}\left\{\frac{1}{1+\mathfrak{a}(\omega)}\right\}\bigg|_{\omega=\lambda_j} = \frac{1}{\mathfrak{a}'(\lambda_j)}, \qquad j = 1, \dots, N/2. \tag{104}$$

It follows that

$$\frac{1}{n!}\int_{\mathcal{C}^n}\left[\prod_{j=1}^n \frac{\mathrm{d}\omega_j}{2\pi\mathrm{i}(1+\mathfrak{a}(\omega_j))}\right] f(\omega_1, \dots, \omega_n) = \sum_{\substack{(\{\lambda^+\},\{\lambda^-\})\in p_2\{\lambda\} \\ |\lambda^+|=n}} \frac{f\left(\lambda_1^+, \dots, \lambda_n^+\right)}{\prod_{j=1}^n \mathfrak{a}'\left(\lambda_j^+\right)}. \tag{105}$$

Below we shall use this formula from the right to the left in order to rewrite sums over partitions as multiple integrals.

In order to apply (105) we split the sum in (99) as

$$\sum_{\substack{(\{\lambda^+\},\{\lambda^-\})\in p_2\{\lambda\} \\ (\{\xi^+\},\{\xi^-\})\in p_2\{\xi\} \\ |\xi^+|+|\lambda^-|=N/2}} = \sum_{n=0}^m \sum_{\substack{(\{\xi^+\},\{\xi^-\})\in p_2\{\xi\} \\ |\xi^+|=n}} \sum_{\substack{(\{\lambda^+\},\{\lambda^-\})\in p_2\{\lambda\} \\ |\lambda^+|=n}}. \tag{106}$$

We would like to apply (105) to the rightmost sum in (106) after inserting it into (99). However, $Y_n(\{\lambda^+\}|\{\xi^+\})Z_n(\{\lambda^+\}|\{\xi^+\}|\{\xi^-\})$ is not analytic in the variables λ_j^+ inside $\mathcal{C}^n$, but for every λ_j^+ has simple poles at $\lambda_j^+ = \xi_k^+$ for $k = 1, \dots, n$ (the function $G(\lambda, \xi)$ has a simple pole at $\lambda = \xi$ (see the appendix), the simple poles of $\det \widetilde{M}\left(\lambda_j^+, \xi_k^+\right)$ at $\lambda_j^+ = \xi_k^+$ are compensated by the simple zeros of $\overline{\mathfrak{b}}\left(\lambda_j^+\right)$). Recall that the ξ_j are free parameters. We choose them distinct from the Bethe roots λ_j and all inside $\mathcal{C}$. Then there is a simple closed contour Γ encircling all the ξ_j but none of the Bethe roots λ_j, and $Y_n(\{\lambda^+\}|\{\xi^+\})Z_n(\{\lambda^+\}|\{\xi^+\}|\{\xi^-\})$ is analytic inside $\mathcal{C} - \Gamma$ (see figure 2). Thus, (105) applies to $\mathcal{C} - \Gamma$, and we obtain

$$\sum_{\substack{(\{\lambda^+\},\{\lambda^-\})\in p_2\{\lambda\}\\ |\lambda^+|=n}} \frac{Y_n(\{\lambda^+\}|\{\xi^+\})Z_n(\{\lambda^+\}|\{\xi^+\}|\{\xi^-\})}{\left[\prod_{j=1}^n \mathfrak{a}'(\lambda_j^+)\right]\left[\prod_{j=1}^{m-n}(1+\mathfrak{a}(\xi_j^-))\right]}$$
$$= \frac{1}{n!}\int_{(\mathcal{C}-\Gamma)^n}\left[\prod_{j=1}^n \frac{\mathrm{d}\omega_j}{2\pi\mathrm{i}(1+\mathfrak{a}(\omega_j))}\right]\left[\prod_{j=1}^{m-n}\frac{1}{(1+\mathfrak{a}(\xi_j^-))}\right]$$
$$\times Y_n\left(\{\omega_j\}_{j=1}^n|\{\xi^+\}\right) Z_n\left(\{\omega_j\}_{j=1}^n\middle|\{\xi^+\}|\{\xi^-\}\right). \tag{107}$$

This is already a multiple integral representation. Note, however, that it is still inappropriate for performing the homogeneous limit and the Trotter limit for two reasons. First, the integrand still contains the auxiliary function $\mathfrak{a}(\xi_j^-)$ which cannot be removed by applying a formula like (105) to the variables ξ_k. But the Trotter limit and the limit $\xi \to 0$ in $\mathfrak{a}(\xi)$ do not commute. Second, since the origin is a limit point of the sequence of Bethe numbers that determine the leading eigenvalue of the quantum transfer matrix in the Trotter limit, we could not avoid that Bethe roots cross the contour Γ if it includes the origin which in turn would be necessary in order to perform the homogeneous limit. The way out of these problems is amazingly straightforward. In the next two sections, we calculate the Γ-integrals explicitly and sum up the resulting terms. In this procedure all unpleasant terms $\mathfrak{a}(\xi_j^-)$ cancel each other.

3.3. *Evaluation of the* Γ*-integrals*

Due to the symmetry in the ω_j of the integrand in (107) we may replace the integral with

$$\int_{(\mathcal{C}-\Gamma)^n}\prod_{j=1}^n \mathrm{d}\omega_j = \sum_{k=0}^n \binom{n}{k}(-1)^k \int_{\mathcal{C}^{n-k}}\left[\prod_{j=1}^{n-k}\mathrm{d}\omega_j\right]\int_{\Gamma^k}\left[\prod_{j=1}^{k}\mathrm{d}\omega_j\right]. \tag{108}$$

Our next task is to evaluate the Γ-integrals. This can be achieved by means of the residue theorem. We obtain the following result,

$$\int_{\Gamma^k}\left[\prod_{j=1}^k \frac{\mathrm{d}\omega_{n-k+j}}{2\pi\mathrm{i}(1+\mathfrak{a}(\omega_{n-k+j}))}\right] Y_n\left(\{\omega_j\}_{j=1}^n\middle|\{\xi^+\}\right) Z_n\left(\{\omega_j\}_{j=1}^n\middle|\{\xi^+\}\middle|\{\xi^-\}\right)$$
$$= k! \sum_{\substack{(\{\xi^{++}\},\{\xi^{+-}\})\in p_2\{\xi^+\}\\ |\xi^{+-}|=k}} Y_{n-k}\left(\{\omega_j\}_{j=1}^{n-k}\middle|\{\xi^{++}\}\right)\left[\prod_{j=1}^k \frac{1}{\left(1+\mathfrak{a}\left(\xi_j^{+-}\right)\right)}\right]$$
$$\times\left[\prod_{j=1}^{m-n}\left(1+\mathrm{e}^{\varphi}\mathfrak{a}(\xi_j^-)\prod_{l=1}^{n-k}\frac{f\left(\xi_j^-,\xi_l^{++}\right)f(\omega_l,\xi_j^-)}{f\left(\xi_l^{++},\xi_j^-\right)f(\xi_j^-,\omega_l)}\right)\right]$$
$$\times\left[\prod_{j=1}^k\left(1-\mathrm{e}^{\varphi}\prod_{l=1}^{n-k}\frac{f\left(\xi_j^{+-},\xi_l^{++}\right)f\left(\omega_l,\xi_j^{+-}\right)}{f\left(\xi_l^{++},\xi_j^{+-}\right)f\left(\xi_j^{+-},\omega_l\right)}\right)\right]. \tag{109}$$

3.4. *Resummation of the* $\mathcal{C}$*-integrals*

Inserting (107)–(109) into (99) we obtain an expression that contains only integrals over the canonical contour $\mathcal{C}$. Yet the summation with respect to the inhomogeneity parameters ξ_j looks more complicated than before. It turns out that these sums can be simplified considerably by applying the following:

Lemma 5. *For any function $F(\xi)$ the identity*

$$\sum_{k=0}^{|\xi|}(-1)^k \sum_{\substack{(\{\xi^+\},\{\xi^-\})\in p_2\{\xi\}\\ |\xi^+|=k}} \left[\prod_{j=1}^{|\xi^-|}(1+\mathrm{e}^{\varphi}\mathfrak{a}(\xi_j^-)F(\xi_j^-))\right]\left[\prod_{j=1}^{|\xi^+|}\big(1-\mathrm{e}^{\varphi}F\big(\xi_j^+\big)\big)\right]$$
$$= \mathrm{e}^{|\xi|\varphi}\prod_{j=1}^{|\xi|}F(\xi_j)(1+\mathfrak{a}(\xi_j)) \tag{110}$$

holds.

Thanks to this lemma we end up with the equation

$$\Phi_N(\varphi|\{\xi\}) = \sum_{n=0}^{m}\frac{\mathrm{e}^{(m-n)\varphi}}{n!}\sum_{\substack{(\{\xi^+\},\{\xi^-\})\in p_2\{\xi\}\\ |\xi^+|=n}}\left[\prod_{j=1}^{n}\frac{1}{\mathfrak{b}'\big(\xi_j^+\big)}\right]$$
$$\times\int_{\mathcal{C}^n}\left[\prod_{j=1}^{n}\frac{\mathrm{d}\omega_j\,\mathfrak{b}(\omega_j)}{2\pi\mathrm{i}(1+\mathfrak{a}(\omega_j))}\right]\left[\prod_{j,k=1}^{n}\frac{\mathrm{sh}\big(\omega_j-\xi_k^+-\eta\big)}{\mathrm{sh}\big(\xi_j^+-\xi_k^+-\eta\big)}\right]$$
$$\times\det M\big(\omega_j,\xi_k^+\big)\det G\big(\omega_j,\xi_k^+\big) \tag{111}$$

for the finite Trotter number approximant to the generating function (35) of the σ^z–σ^z correlation functions. Here we introduced the new abbreviations

$$\mathfrak{b}(\lambda) = \prod_{k=1}^{m}\frac{1}{f(\xi_k,\lambda)}, \tag{112}$$

$$M\big(\omega_j,\xi_k^+\big) = t\big(\xi_k^+,\omega_j\big)\prod_{l=1}^{n}\frac{\mathrm{sh}\big(\omega_j-\xi_l^+-\eta\big)}{\mathrm{sh}(\omega_j-\omega_l-\eta)} + t\big(\omega_j,\xi_k^+\big)\,\mathrm{e}^{\varphi}\prod_{l=1}^{n}\frac{\mathrm{sh}\big(\omega_j-\xi_l^++\eta\big)}{\mathrm{sh}(\omega_j-\omega_l+\eta)}. \tag{113}$$

The integral on the right-hand side of (111) is analytic and symmetric in the ξ_j^+ inside $\mathcal{C}^n$. It vanishes if any two of the ξ_j are identical. The function $1/\mathfrak{b}(\lambda)$ is meromorphic inside $\mathcal{C}$ with only simple poles located at $\lambda=\xi_j$. Hence, we can apply (105) to any simple closed contour Γ which lies inside $\mathcal{C}$ and encircles all the inhomogeneities ξ_j. It follows that

$$\Phi_N(\varphi|\{\xi\}) = \sum_{n=0}^{m}\frac{\mathrm{e}^{(m-n)\varphi}}{(n!)^2}\left[\prod_{j=1}^{n}\int_\Gamma\frac{\mathrm{d}\zeta_j}{2\pi\mathrm{i}\mathfrak{b}(\zeta_j)}\int_{\mathcal{C}}\frac{\mathrm{d}\omega_j\,\mathfrak{b}(\omega_j)}{2\pi\mathrm{i}(1+\mathfrak{a}(\omega_j))}\right]$$
$$\times\left[\prod_{j,k=1}^{n}\frac{\mathrm{sh}(\omega_j-\zeta_k-\eta)}{\mathrm{sh}(\zeta_j-\zeta_k-\eta)}\right]\det M(\omega_j,\zeta_k)\det G(\omega_j,\zeta_k). \tag{114}$$

This is our final formula for the finite Trotter number approximant $\Phi_N(\varphi|\{\xi\})$. We are now in a position to take the homogeneous limit and the Trotter limit analytically.

3.5. Taking the limits

The information about the inhomogeneities is contained in the function $\mathfrak{b}(\lambda)$. From its definition we see immediately that

$$\lim_{\xi_1,\dots,\xi_m\to 0}\mathfrak{b}(\lambda) = \left(\frac{\mathrm{sh}(\lambda)}{\mathrm{sh}(\lambda-\eta)}\right)^m. \tag{115}$$

The information about the discreteness of the Trotter decomposition, on the other hand, is implicit in the function $\mathfrak{a}(\lambda)$. Taking the Trotter limit means taking $\mathfrak{a}(\lambda)$ as a solution of equation (63). Thus, we conclude and summarize our main result.

Theorem. *The generating function of the σ^z–σ^z correlation functions of the XXZ chain has the following integral representation,*

$$\left\langle \exp\left\{\varphi\sum_{n=1}^{m} e_{n\,2}^{\,2}\right\}\right\rangle_{T,h} = \sum_{n=0}^{m}\frac{\mathrm{e}^{(m-n)\varphi}}{(n!)^2}\left[\prod_{j=1}^{n}\int_\Gamma\frac{\mathrm{d}\zeta_j}{2\pi\mathrm{i}}\left(\frac{\mathrm{sh}(\zeta_j-\eta)}{\mathrm{sh}(\zeta_j)}\right)^m\int_{\mathcal{C}}\frac{\mathrm{d}\omega_j}{2\pi\mathrm{i}(1+\mathfrak{a}(\omega_j))}\left(\frac{\mathrm{sh}(\omega_j)}{\mathrm{sh}(\omega_j-\eta)}\right)^m\right] \times\left[\prod_{j,k=1}^{n}\frac{\mathrm{sh}(\omega_j-\zeta_k-\eta)}{\mathrm{sh}(\zeta_j-\zeta_k-\eta)}\right]\det M(\omega_j,\zeta_k)\det G(\omega_j,\zeta_k), \tag{116}$$

where $\mathfrak{a}(\lambda)$ is the auxiliary function (63) that determines the free energy in the Trotter limit,

$$M(\omega_j,\zeta_k) = t(\zeta_k,\omega_j)\prod_{l=1}^{n}\frac{\mathrm{sh}(\omega_j-\zeta_l-\eta)}{\mathrm{sh}(\omega_j-\omega_l-\eta)} + t(\omega_j,\zeta_k)\,\mathrm{e}^{\varphi}\prod_{l=1}^{n}\frac{\mathrm{sh}(\omega_j-\zeta_l+\eta)}{\mathrm{sh}(\omega_j-\omega_l+\eta)}, \tag{117}$$

and the function $G(\lambda,\zeta)$ is the solution of the linear integral equation

$$G(\lambda,\zeta) = t(\zeta,\lambda) + \int_{\mathcal{C}}\frac{\mathrm{d}\omega}{2\pi\mathrm{i}}\frac{\mathrm{sh}(2\eta)}{\mathrm{sh}(\lambda-\omega+\eta)\,\mathrm{sh}(\lambda-\omega-\eta)}\frac{G(\omega,\zeta)}{1+\mathfrak{a}(\omega)}. \tag{118}$$

The contour $\mathcal{C}$ is the canonical contour in the non-linear integral equation formalism (see figure 1). Γ is any simple closed contour which lies inside $\mathcal{C}$ and encircles the origin.

As we have seen in sections 2.7 and 2.8 both auxiliary functions, $\mathfrak{a}$ and $\overline{\mathfrak{a}}$, can be equivalently used to express physical quantities. To switch from one representation to the other one can use the identity

$$\frac{1}{1+\mathfrak{a}(\lambda)} = 1 - \frac{1}{1+\overline{\mathfrak{a}}(\lambda)}. \tag{119}$$

Inserting it into (118) and using

$$\frac{\mathrm{sh}(2\eta)}{\mathrm{sh}(\lambda-\zeta+\eta)\,\mathrm{sh}(\lambda-\zeta-\eta)} = t(\lambda,\zeta)+t(\zeta,\lambda) \tag{120}$$

we find, for instance,

$$G(\lambda,\zeta) = -t(\lambda,\zeta) - \int_{\mathcal{C}}\frac{\mathrm{d}\omega}{2\pi\mathrm{i}}\frac{\mathrm{sh}(2\eta)}{\mathrm{sh}(\lambda-\omega+\eta)\,\mathrm{sh}(\lambda-\omega-\eta)}\frac{G(\omega,\zeta)}{1+\overline{\mathfrak{a}}(\omega)} \tag{121}$$

which equally well defines the inhomogeneous density function $G(\lambda,\zeta)$. The task of re-expressing the multiple integral representation (116) in terms of $\overline{\mathfrak{a}}$ is, of course, more cumbersome. One may, for instance, start from (114), insert (119), evaluate the integrals which do not contain $\overline{\mathfrak{a}}$, and resum the resulting terms in a similar way as in section 3.4. One arrives at the following:

Corollary. *When expressed in terms of* $\overline{\mathfrak{a}}$ *the generating function takes the form*

$$\left\langle \exp\left\{\varphi\sum_{n=1}^{m} e_{n}{}^{2}_{2}\right\}\right\rangle_{T,h} = \sum_{n=0}^{m}\frac{(-1)^n}{(n!)^2}\left[\prod_{j=1}^{n}\int_\Gamma\frac{\mathrm{d}\zeta_j}{2\pi\mathrm{i}}\left(\frac{\mathrm{sh}(\zeta_j+\eta)}{\mathrm{sh}(\zeta_j)}\right)^m\int_C\frac{\mathrm{d}\omega_j}{2\pi\mathrm{i}(1+\overline{\mathfrak{a}}(\omega_j))}\left(\frac{\mathrm{sh}(\omega_j)}{\mathrm{sh}(\omega_j+\eta)}\right)^m\right] \times\left[\prod_{j,k=1}^{n}\frac{\mathrm{sh}(\omega_j-\zeta_k+\eta)}{\mathrm{sh}(\zeta_j-\zeta_k+\eta)}\right]\det M(\omega_j,\zeta_k)\det G(\omega_j,\zeta_k), \tag{122}$$

where $M(\omega_j,\zeta_k)$ *and* $G(\omega_j,\zeta_k)$ *are the same as in theorem 1.*

In the remaining sections we shall discuss several special cases and limits of (116) and (122).

3.6. One-point function

We begin with the one-point function obtained from (116) or (122), respectively, for $m = 1$. In this case the sums on the right-hand side of (116) and (122) consist of only two terms, the first of which does not contain any integral. In the second term the integration over Γ can easily be performed, and one remains with the formulae

$$\left\langle\begin{pmatrix}1 & 0\\ 0 & e^{\varphi}\end{pmatrix}_1\right\rangle_{T,h} = \mathrm{e}^{\varphi} - (1-\mathrm{e}^{\varphi})\int_C\frac{\mathrm{d}\omega}{2\pi\mathrm{i}}\frac{G(\omega)}{1+\mathfrak{a}(\omega)} = 1 + (1-\mathrm{e}^{\varphi})\int_C\frac{\mathrm{d}\omega}{2\pi\mathrm{i}}\frac{G(\omega)}{1+\overline{\mathfrak{a}}(\omega)}. \tag{123}$$

Here we inserted the identity $G(\omega) = G(\omega, 0)$ which is obtained by comparing (72) and (118).

Setting $\varphi = 0$ in the above equation both expressions for the one-point function yield 1 as it has to be. Setting $\varphi = \mathrm{i}\pi$, on the other hand, and multiplying (123) by 1/2 we obtain two formulae for the magnetization,

$$\langle S_1^z\rangle_{T,h} = -\frac{1}{2} - \int_C\frac{\mathrm{d}\omega}{2\pi\mathrm{i}}\frac{G(\omega)}{1+\mathfrak{a}(\omega)} = \frac{1}{2} + \int_C\frac{\mathrm{d}\omega}{2\pi\mathrm{i}}\frac{G(\omega)}{1+\overline{\mathfrak{a}}(\omega)}. \tag{124}$$

These formulae are the same as obtained in section 2.8 based on a completely different reasoning, namely by taking the derivative of the free energy with respect to the magnetic field.

3.7. Emptiness formation probability

In the limiting cases $\varphi \to \pm\infty$ (for $\varphi \to \infty$ one has to multiply by $\mathrm{e}^{-m\varphi}$ first in order to obtain a finite result) our formulae (116) and (122) simplify considerably. The resulting expressions on the left-hand side of (116) and (122), $\langle e_1{}^1_1 \dots e_m{}^1_1\rangle_{T,h}$ or $\langle e_1{}^2_2 \dots e_m{}^2_2\rangle_{T,h}$, respectively, describe the probability to find a string of up- or down-spins of length m. For spin chains these probabilities were introduced in [13]. They are named the 'emptiness formation probability' and recently became popular, since the integrals in the zero temperature multiple integral representation of the emptiness formation probability [4, 13] could be evaluated explicitly for small m [1].

For finite temperatures our formulae (116) and (122) yield the two alternative expressions

$$\langle e_1{}^1_1 \dots e_m{}^1_1\rangle_{T,h} = \frac{1}{(m!)^2}\left[\prod_{j=1}^{m}\int_\Gamma\frac{\mathrm{d}\zeta_j}{2\pi\mathrm{i}}\left(\frac{\mathrm{sh}(\zeta_j-\eta)}{\mathrm{sh}(\zeta_j)}\right)^m\int_C\frac{\mathrm{d}\omega_j}{2\pi\mathrm{i}(1+\mathfrak{a}(\omega_j))}\left(\frac{\mathrm{sh}(\omega_j)}{\mathrm{sh}(\omega_j-\eta)}\right)^m\right]$$

$$\times \left[\prod_{j,k=1}^{n} \frac{\operatorname{sh}^2(\omega_j - \zeta_k - \eta)}{\operatorname{sh}(\zeta_j - \zeta_k - \eta) \operatorname{sh}(\omega_j - \omega_k - \eta)} \right] \det\, t(\zeta_k, \omega_j) \det G(\omega_j, \zeta_k) \tag{125a}$$

$$= \sum_{n=0}^{m} \frac{(-1)^n}{(n!)^2} \left[\prod_{j=1}^{n} \int_\Gamma \frac{\mathrm{d}\zeta_j}{2\pi \mathrm{i}} \left(\frac{\operatorname{sh}(\zeta_j + \eta)}{\operatorname{sh}(\zeta_j)} \right)^m \int_{\mathcal{C}} \frac{\mathrm{d}\omega_j}{2\pi \mathrm{i}(1 + \overline{\mathfrak{a}}(\omega_j))} \left(\frac{\operatorname{sh}(\omega_j)}{\operatorname{sh}(\omega_j + \eta)} \right)^m \right]$$

$$\times \left[\prod_{j,k=1}^{n} \frac{\operatorname{sh}(\omega_j - \zeta_k + \eta) \operatorname{sh}(\omega_j - \zeta_k - \eta)}{\operatorname{sh}(\zeta_j - \zeta_k + \eta) \operatorname{sh}(\omega_j - \omega_k - \eta)} \right] \det\, t(\zeta_k, \omega_j) \det G(\omega_j, \zeta_k) \tag{125b}$$

for $\langle e_{1}{}_{1}^{1} \dots e_{m}{}_{1}^{1} \rangle_{T,h}$ and, similarly,

$$\langle e_{1}{}_{2}^{2} \dots e_{m}{}_{2}^{2} \rangle_{T,h}$$

$$= \frac{(-1)^m}{(m!)^2} \left[\prod_{j=1}^{m} \int_\Gamma \frac{\mathrm{d}\zeta_j}{2\pi \mathrm{i}} \left(\frac{\operatorname{sh}(\zeta_j + \eta)}{\operatorname{sh}(\zeta_j)} \right)^m \int_{\mathcal{C}} \frac{\mathrm{d}\omega_j}{2\pi \mathrm{i}(1 + \overline{\mathfrak{a}}(\omega_j))} \left(\frac{\operatorname{sh}(\omega_j)}{\operatorname{sh}(\omega_j + \eta)} \right)^m \right]$$

$$\times \left[\prod_{j,k=1}^{n} \frac{\operatorname{sh}^2(\omega_j - \zeta_k + \eta)}{\operatorname{sh}(\zeta_j - \zeta_k + \eta) \operatorname{sh}(\omega_j - \omega_k + \eta)} \right] \det t(\omega_j, \zeta_k) \det G(\omega_j, \zeta_k) \tag{126a}$$

$$= \sum_{n=0}^{m} \frac{1}{(n!)^2} \left[\prod_{j=1}^{n} \int_\Gamma \frac{\mathrm{d}\zeta_j}{2\pi \mathrm{i}} \left(\frac{\operatorname{sh}(\zeta_j - \eta)}{\operatorname{sh}(\zeta_j)} \right)^m \int_{\mathcal{C}} \frac{\mathrm{d}\omega_j}{2\pi \mathrm{i}(1 + \mathfrak{a}(\omega_j))} \left(\frac{\operatorname{sh}(\omega_j)}{\operatorname{sh}(\omega_j - \eta)} \right)^m \right]$$

$$\times \left[\prod_{j,k=1}^{n} \frac{\operatorname{sh}(\omega_j - \zeta_k + \eta) \operatorname{sh}(\omega_j - \zeta_k - \eta)}{\operatorname{sh}(\zeta_j - \zeta_k + \eta) \operatorname{sh}(\omega_j - \omega_k - \eta)} \right] \det\, t(\omega_j, \zeta_k) \det G(\omega_j, \zeta_k). \tag{126b}$$

3.8. Zero temperature limit

How can we make contact with the zero temperature results obtained in [5]? It is clear by inspection that the auxiliary functions $\mathfrak{a}$ and $\overline{\mathfrak{a}}$ defined by (63) and (65) do not approach a limit as T goes to zero. The inhomogeneities are unbounded in T. In order to obtain a sensible result we have to multiply by T first. Setting $\varepsilon(\lambda) = -T \ln(\mathfrak{a}(\lambda)) = T \ln(\overline{\mathfrak{a}}(\lambda))$ the non-linear integral equations turn into

$$\varepsilon(\lambda) = h + \frac{2J \operatorname{sh}^2(\eta)}{\operatorname{sh}(\lambda) \operatorname{sh}(\lambda + \eta)} + \int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi \mathrm{i}} \frac{\operatorname{sh}(2\eta) T \ln(1 + \mathrm{e}^{-\varepsilon(\omega)/T})}{\operatorname{sh}(\lambda - \omega + \eta) \operatorname{sh}(\lambda - \omega - \eta)} \tag{127a}$$

$$= h - \frac{2J \operatorname{sh}^2(\eta)}{\operatorname{sh}(\lambda) \operatorname{sh}(\lambda - \eta)} + \int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi \mathrm{i}} \frac{\operatorname{sh}(2\eta) T \ln(1 + \mathrm{e}^{\varepsilon(\omega)/T})}{\operatorname{sh}(\lambda - \omega + \eta) \operatorname{sh}(\lambda - \omega - \eta)}. \tag{127b}$$

Here we shift the left and right edges of the integration contour to $\pm\eta/2$, where $\varepsilon(\lambda)$ is real (recall that the contributions from the upper and the lower edge cancel each other). We see that it only matters if $\varepsilon(\lambda)$ is positive or negative as T goes to zero. In (127a) only the negative part of $\varepsilon(\lambda)$ on the contour contributes to the zero temperature limit, in (127*b*) only the positive part. This divides the contour $\mathcal{C}$ into two disjoint pieces $\mathcal{C}^{(+)}$ and $\mathcal{C}^{(-)}$ on which $\varepsilon(\lambda)$ can be calculated by means of the linear integral equations

$$\varepsilon(\lambda) = h + \frac{2J\,\mathrm{sh}^2(\eta)}{\mathrm{sh}(\lambda)\,\mathrm{sh}(\lambda+\eta)} - \int_{\mathcal{C}^{(-)}} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{\mathrm{sh}(2\eta)\varepsilon(\omega)}{\mathrm{sh}(\lambda-\omega+\eta)\,\mathrm{sh}(\lambda-\omega-\eta)}, \tag{128a}$$

$$\varepsilon(\lambda) = h - \frac{2J\,\mathrm{sh}^2(\eta)}{\mathrm{sh}(\lambda)\,\mathrm{sh}(\lambda-\eta)} + \int_{\mathcal{C}^{(+)}} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{\mathrm{sh}(2\eta)\varepsilon(\omega)}{\mathrm{sh}(\lambda-\omega+\eta)\,\mathrm{sh}(\lambda-\omega-\eta)}. \tag{128b}$$

These integral equations can be transformed into integral equations for dressed energies, which is, however, not our actual aim. The most important conclusion instead is that

$$\frac{1}{1+\overline{\mathfrak{a}}(\lambda)} = \frac{1}{1+\mathrm{e}^{\varepsilon(\lambda)/T}} \quad \xrightarrow{T\to 0} \quad \begin{cases} 0 & \text{on } \mathcal{C}^{(+)} \\ 1 & \text{on } \mathcal{C}^{(-)} \end{cases}. \tag{129}$$

This function behaves like a 'Fermi function on $\mathcal{C}$'.

Applying (129) to the integral equation (121) and shifting the arguments appropriately we obtain

$$-G\left(\lambda-\frac{\eta}{2},\zeta-\frac{\eta}{2}\right) - \int_{\mathcal{C}^{(-)}+\frac{\eta}{2}} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{\mathrm{sh}(2\eta)G\left(\omega-\frac{\eta}{2},\zeta-\frac{\eta}{2}\right)}{\mathrm{sh}(\lambda-\omega+\eta)\,\mathrm{sh}(\lambda-\omega-\eta)} = t(\lambda,\zeta). \tag{130}$$

This equation has to be compared with equation (2.16) of [5]. The two equations agree if we set

$$G\left(\lambda-\frac{\eta}{2},\zeta-\frac{\eta}{2}\right) = 2\pi\mathrm{i}\rho(\lambda,\zeta) \tag{131}$$

and identify the integration contour in equation (2.16) of [5] with $-\left(\mathcal{C}^{(-)}+\frac{\eta}{2}\right)$. A close inspection (for details see, e.g., [10]) of (127) and (128) shows indeed that (for $h>0$, $\eta<0$!) the contour $\mathcal{C}^{(-)}$ is a line segment $\mathrm{Re}\,\lambda = \eta/2$, $-\alpha < \mathrm{Im}\,\lambda < \alpha$ (where $\alpha>0$ depends on the magnetic field h). This is sufficient to identify (130) with (2.16) of [5].

Let us introduce the shorthand notation $\mathcal{I} = -\left(\mathcal{C}^{(-)}+\frac{\eta}{2}\right)$. Then, using (129) and (131), our second expression (122) for the generating function of the σ^z–σ^z correlation functions can be evaluated in the zero temperature limit. We obtain

$$\begin{aligned}\lim_{T\to 0}\left\langle \exp\left\{\varphi\sum_{n=1}^{m} e^{2}_{n2}\right\}\right\rangle_{T,h} &= \sum_{n=0}^{m}\frac{1}{(n!)^2}\left[\prod_{j=1}^{n}\int_{\Gamma+\frac{\eta}{2}}\frac{\mathrm{d}\zeta_j}{2\pi\mathrm{i}}\left(\frac{\mathrm{sh}\left(\zeta_j+\frac{\eta}{2}\right)}{\mathrm{sh}\left(\zeta_j-\frac{\eta}{2}\right)}\right)^m\int_{\mathcal{I}}\mathrm{d}\omega_j\left(\frac{\mathrm{sh}\left(\omega_j-\frac{\eta}{2}\right)}{\mathrm{sh}\left(\omega_j+\frac{\eta}{2}\right)}\right)^m\right] \\ &\quad\times\left[\prod_{j,k=1}^{n}\frac{\mathrm{sh}(\omega_j-\zeta_k+\eta)}{\mathrm{sh}(\zeta_j-\zeta_k+\eta)}\right]\det M(\omega_j,\zeta_k)\det\rho(\omega_j,\zeta_k),\end{aligned} \tag{132}$$

where $\rho(\lambda,\zeta)$ is the solution of the linear integral equation

$$-2\pi\mathrm{i}\rho(\lambda,\zeta) + \int_{\mathcal{I}}\mathrm{d}\omega\frac{\mathrm{sh}(2\eta)\rho(\omega,\zeta)}{\mathrm{sh}(\lambda-\omega+\eta)\,\mathrm{sh}(\lambda-\omega-\eta)} = t(\lambda,\zeta) \tag{133}$$

which is precisely the result of [5].

3.9. High temperature limit

In the limit of infinite temperature all correlations should vanish. How can this be seen from our formulae? For $T \to \infty$ the inhomogeneity on the right-hand side of the integral equations (63) and (65) vanishes. The remaining homogeneous equations are solved by $\mathfrak{a}(\lambda) = 1$ or $\overline{\mathfrak{a}}(\lambda) = 1$, respectively. Inserting this, for instance, into (116) we see that the only singularities in the resulting integrand are the simple poles of the function $G(\omega, \zeta)$. Therefore the integrals can be calculated by means of the residue theorem. Using similar techniques as described in section 3.4 we can simplify the result which finally turns into

$$\lim_{T\to\infty} \left\langle \exp\left\{\varphi \sum_{n=1}^{m} e_{n\,2}^{\,2}\right\}\right\rangle_{T,h} = \left(\frac{1+\mathrm{e}^{\varphi}}{2}\right)^{m}. \tag{134}$$

Applying (36) we obtain

$$\lim_{T\to\infty} \langle \sigma_1^z \sigma_m^z \rangle_{T,h} = 0 \tag{135}$$

as we expected.

4. Conclusions

In this work, integral representations for finite temperature correlation functions of an integrable model have been derived for the first time. We concentrated on the generating function (35) of the σ^z–σ^z correlation functions, since it appeared particularly appropriate to us for developing the method. Now this method may be applied to other generating functions and also directly to two-point functions. Work in this direction is underway.

It will be very interesting to study the integral representations further. How can they be utilized to obtain the long-distance asymptotics? How efficient are they for numerical calculations? Are there special cases where part of the integrations can be performed analytically? We hope to address these questions in forthcoming publications.

We restricted our presentation to the off-critical regime $\Delta > 1$. We would like to stress, however, that our results straightforwardly extend to the critical regime $|\Delta| \leqslant 1$, where only the canonical contour has to be redefined (see figure 3).

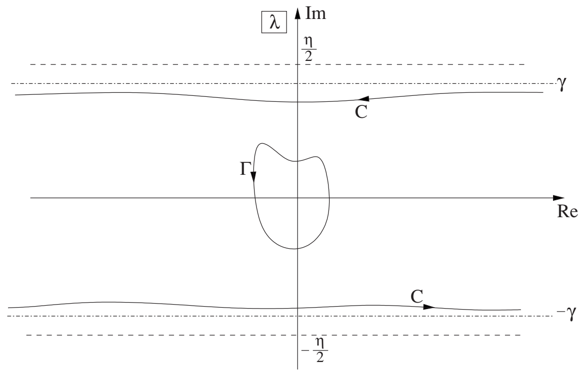

Figure 3. Contours of integration in the critical regime for $0 \leqslant \Delta < 1$. For $-1 < \Delta \leqslant 0$ one has to choose $|\gamma| < \frac{\pi}{2} - \frac{|\eta|}{2}$. Alternatively one may switch the sign of J making use of the equivalence of the parameter regimes $-1\Delta \leqslant 0$, $J < 0$ and $0 \leqslant \Delta < 1$, $J < 0$.

The situation is much the same as in the zero temperature limit [25].

Acknowledgment

The authors would like to thank M Karbach for helpful discussions.

Appendix. A ratio of determinants

Here we prove lemma 3. We define a column vector $\mathbf{n}(\xi)$ with entries

$$\mathbf{n}_j(\xi) = t(\tilde{\lambda}_j, \xi) - t(\xi, \tilde{\lambda}_j)\mathfrak{a}(\xi), \qquad j = 1, \ldots, N/2 \tag{A.1}$$

and another column vector

$$\mathbf{j}(\xi) = N_0^{-1}\,\mathbf{n}(\xi). \tag{A.2}$$

The matrices N_0 and N_n have the last $N/2 - n$ columns in common. Thus, we conclude that

$$\frac{\det N_n}{\det N_0} = \det N_0^{-1} N_n = \det(\mathbf{j}(\tilde{\xi}_1), \ldots, \mathbf{j}(\tilde{\xi}_n), \mathbf{e}_{n+1}, \ldots, \mathbf{e}_{N/2}) = \det\langle \mathbf{e}_j, \mathbf{j}(\tilde{\xi}_k)\rangle, \tag{A.3}$$

where the $\mathbf{e}_j$ are the canonical unit column vectors having a single non-zero entry 1 in the jth row, and j and k on the right-hand side run from 1 to n. In (A.3) we have expressed the ratio of two $N/2 \times N/2$ determinants as a single $n \times n$ determinant, a trick we borrowed from [6].

In the second step of our proof we transform the equation $N_0\,\mathbf{j}(\xi) = \mathbf{n}(\xi)$ that determines $\mathbf{j}$ into an integral equation. For this purpose, we first of all rewrite it in components,

$$-\mathfrak{a}'(\tilde{\lambda}_k)\,\mathbf{j}_k(\xi) + \sum_{l=1}^{N/2} \frac{\operatorname{sh}(2\eta)\,\mathbf{j}_l(\xi)}{\operatorname{sh}(\tilde{\lambda}_k - \tilde{\lambda}_l + \eta)\operatorname{sh}(\tilde{\lambda}_k - \tilde{\lambda}_l - \eta)} = t(\tilde{\lambda}_k, \xi) - t(\xi, \tilde{\lambda}_k)\mathfrak{a}(\xi). \tag{A.4}$$

We define a function

$$F(\lambda, \xi) = t(\xi, \lambda)\mathfrak{a}(\xi) - t(\lambda, \xi) + \sum_{l=1}^{N/2} \frac{\operatorname{sh}(2\eta)\,\mathbf{j}_l(\xi)}{\operatorname{sh}(\lambda - \tilde{\lambda}_l + \eta)\operatorname{sh}(\lambda - \tilde{\lambda}_l - \eta)} \tag{A.5}$$

and observe that this function determines $\mathbf{j}(\xi)$ through

$$F(\tilde{\lambda}_k, \xi) = \mathfrak{a}'(\tilde{\lambda}_k)\,\mathbf{j}_k(\xi). \tag{A.6}$$

We shall now assume that ξ is located inside our canonical contour $\mathcal{C}$ sketched in figure 1. Then the only singularity of $F(\lambda, \xi)$ as a function of λ inside the rectangle Q (see again figure 1) is a simple pole at $\lambda = \xi$. The residue at this pole is

$$\operatorname{res}\{F(\lambda, \xi)\}|_{\lambda=\xi} = \lim_{\lambda\to\xi} \operatorname{sh}(\lambda - \xi)F(\lambda, \xi) = -1 - \mathfrak{a}(\xi). \tag{A.7}$$

This residue gives an additional contribution when we apply equation (105) to (A.5) in order to transform the sum on the right-hand side into an integral. We end up with

$$F(\lambda, \xi) = t(\xi, \lambda)(1 + \mathfrak{a}(\xi)) + \int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{\operatorname{sh}(2\eta)}{\operatorname{sh}(\lambda - \omega + \eta)\operatorname{sh}(\lambda - \omega - \eta)} \frac{F(\omega, \xi)}{1 + \mathfrak{a}(\omega)}. \tag{A.8}$$

The latter equation suggests to introduce a function

$$G(\lambda, \xi) = \frac{F(\lambda, \xi)}{1 + \mathfrak{a}(\xi)}. \tag{A.9}$$

This function then solves the linear integral equation (97) defined in lemma 3. Coming back to our original notation (see (93)) we may finally express the ratio of the two determinants as

$$\frac{\det N_n}{\det N_0} = \left[\prod_{l=1}^{n} \frac{1 + \mathfrak{a}\big(\xi_l^+\big)}{\mathfrak{a}'\big(\lambda_l^+\big)}\right] \det G\big(\lambda_j^+, \xi_k^+\big), \tag{A.10}$$

and our lemma is proved.

Note that it follows from (A.7) and (A.9) that the only singularity of $G(\lambda, \xi)$ (considered as a function of λ) inside the rectangle Q is a simple pole with residue -1 at $\lambda = \xi$. This fact is frequently used in the derivation of the multiple integral representations (116) and (122).

References

[1] 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

[2] Gaudin M 1983 *La fonction de l'onde de Bethe pour les modèles exacts de la méchanique statistique* (Paris: Masson)

[3] Izergin A G and Korepin V E 1984 The quantum inverse scattering method approach to correlation-functions *Commun. Math. Phys.* **94** 67

[4] Jimbo M, Miki K, Miwa T and Nakayashiki A 1992 Correlation functions of the *XXZ* model for $\Delta < -1$ *Phys. Lett.* A **168** 256

[5] Kitanine N, Maillet J M, Slavnov N A and Terras V 2002 Spin–spin correlation functions of the *XXZ*-$\frac{1}{2}$ Heisenberg chain in a magnetic field *Nucl. Phys.* B **641** 487

[6] 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

[7] Klümper A 1992 Free energy and correlation length of quantum chains related to restricted solid-on-solid lattice models *Ann. Phys., Lpz.* **1** 540

[8] Klümper A 1993 Thermodynamics of the anisotropic spin-1/2 Heisenberg chain and related quantum chains *Z. Phys.* B **91** 507

[9] Schollwöck U, Richter J, Farnell D J J and Bishop R F 2004 Quantum magnetism *Lecture Notes in Physics* vol 645 (Berlin: Springer) p 478

[10] Klümper A and Scheeren C 2003 The thermodynamics of the spin-$\frac{1}{2}$ *XXX* chain: free energy and low-temperature singularities of correlation lengths *Classical and Quantum Nonlinear Integrable Systems: Theory and Application* ed A Kundu (Beogard: Institute of Physics)

[11] Korepin V E 1982 Calculation of norms of Bethe wave functions *Commun. Math. Phys.* **86** 391

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

[13] Korepin V E, Izergin A G, Essler F H L and Uglov D B 1994 Correlation function of the spin-$\frac{1}{2}$ *XXX* antiferromagnet *Phys. Lett.* A **190** 182

[14] Sklyanin E K 1995 Separation of variables—new trends *Prog. Theor. Phys. Suppl.* **118** 35

[15] Slavnov N A 1989 Calculation of scalar products of the wave functions and form factors in the framework of the algebraic Bethe ansatz *Teor. Mat. Fiz.* **79** 232

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

[17] 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

[18] Takahashi M 1999 *Thermodynamics of One-Dimensional Solvable Models* (Cambridge: Cambridge University Press)