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Surface free energy for systems with integrable boundary conditions

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Abstract

The surface free energy is the difference between the free energies for a system with open boundary conditions and the same system with periodic boundary conditions. We use the quantum transfer matrix formalism to express the surface free energy in the thermodynamic limit of systems with integrable boundary conditions as a matrix element of certain projection operators. Specializing to the XXZ spin-1/2 chain we introduce a novel 'finite temperature boundary operator' which characterizes the thermodynamical properties of surfaces related to integrable boundary conditions.

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1. Introduction

The embedding of non-magnetic impurities into spin chains has profound effects on the low-energy properties of such systems. Quantities such as the magnetic susceptibility will acquire corrections of order $\mathcal{O}(L^0)$ which are directly accessible to experimental observation (L being the length of the chains). The dependence of these surface contributions on temperature and magnetic field has been a focus of theoretical work for some time now. Apart from field theoretical approaches [7, 8] the exact solution of the XXZ spin-1/2 chain with open boundary conditions [1, 17] has been used to address this problem [4, 6, 22]. At zero temperature, the calculation of surface contributions to the ground state energy and the magnetic susceptibilities by means of the Bethe ansatz is well established [2, 3, 6, 12, 22]. For finite T, bulk thermal properties are known from the thermodynamic Bethe ansatz (TBA) based on the so-called string hypothesis [20]. This approach has been extended to compute surface corrections to these quantities [4, 6, 22]. The temperature dependence of the boundary susceptibility obtained

this way, however, disagrees with the field theoretical results [7, 8] which, when combined with the leading $T = 0$ contribution from the Bethe ansatz, have been shown to provide the correct low-temperature asymptotics [3]. In addition, this approach fails to reproduce the correct high-temperature behaviour. Since the Bethe ansatz yields reliable results for the open chains at $T = 0$, the origin of these problems is likely to be the improper treatment of the combinatoric entropy which is a central quantity in the TBA. First attempts to extend the TBA for the calculation of the surface contributions to the free energy exist [21]. It is still an open issue, though, whether this approach can resolve the problems mentioned above.

In this paper we choose a different approach to obtain the surface contribution to the free energy from the exact solution by combining Sklyanin's work [17] on the algebraic construction of integrable open boundary conditions with the quantum transfer matrix approach [15, 16, 18, 19] to the thermodynamics of solvable quantum systems in one dimension.

In section 2 we recall the results of Sklyanin's work [17] as far as they are needed for our purposes. Section 3 contains a short review of the quantum transfer matrix approach to the thermodynamics of solvable quantum lattice models. In spirit and notation we follow [9], where more details can be found. Section 4 contains our first expression for the surface free energy of a system connected to Sklyanin's reflection algebra and treatable by the quantum transfer matrix method. The formula is exposed in proposition 4 and shows how to obtain the surface free energy as a Trotter limit of an expectation value of a product of certain projection operators which are local in the space where the quantum transfer matrix acts. The expectation value is taken in a certain so-called dominant eigenstate of the quantum transfer matrix. A second expression for the surface free energy as an expectation value of a non-local operator in the dominant state is derived in section 5 (see equation (66)). Again a Trotter limit must be taken, and a novel 'finite temperature boundary operator' appears. From its properties, worked out in the remainder of section 5, we shall see that it is a generic object in the context of the quantum transfer matrix formalism applied to open boundary systems. From section 5 on we restrict ourselves to the example of the XXZ chain with local spins $\frac{1}{2}$ and only comment on the generalization of the results later in the concluding section 6.

2. Integrable boundary conditions

Our construction of the finite temperature boundary operator is based on a combination of the quantum transfer matrix approach to the thermodynamics of 'Yang–Baxter integrable' systems, as reviewed in the following section, with Sklyanin's work [17] on the construction of integrable boundary conditions. Sklyanin's construction is valid for a fairly general class of integrable systems characterized by an R-matrix of the form $R(\lambda, \mu) = R(\lambda - \mu) \in \mathrm{End}(V \otimes V)$ (V vector space with $\dim V = d \in \mathbb{N}$) which not only satisfies the Yang–Baxter equation

$$R_{12}(\lambda, \mu)R_{13}(\lambda, \nu)R_{23}(\mu, \nu) = R_{23}(\mu, \nu)R_{13}(\lambda, \nu)R_{12}(\lambda, \mu) \tag{1}$$

but also several additional conditions. Namely, $R(\lambda)$ is symmetric in the sense that

$$PR(\lambda)P = R(\lambda), \tag{2}$$

where P is the transposition map on $V \otimes V$ ($Px \otimes y = y \otimes x$). Furthermore, $R(\lambda)$ is unitary,

$$R(\lambda)R(-\lambda) = \rho(\lambda) \tag{3}$$

for some complex function $\rho(\lambda)$, and crossing unitary,

$$R^{t_1}(\lambda)R^{t_1}(-\lambda - 2\eta) = \tilde{\rho}(\lambda) \tag{4}$$

for another complex function $\tilde{\rho}(\lambda)$ and η is a parameter characterizing the R-matrix. The superscript t_1 in (4) denotes the transposition with respect to the first space in the tensor product $V \otimes V$. Similarly, t_2 will denote the transposition with respect to the second space. Then $R(\lambda)$ is a symmetric matrix if

$$R^{t_1 t_2}(\lambda) = R(\lambda) \quad \Leftrightarrow \quad R^{t_1}(\lambda) = R^{t_2}(\lambda), \tag{5}$$

which is also assumed by Sklyanin.

Example. Our chief example will be the R-matrix

$$R(\lambda) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & b(\lambda) & c(\lambda) & 0 \\ 0 & c(\lambda) & b(\lambda) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{6}$$

with

$$b(\lambda) = \frac{\mathrm{sh}(\lambda)}{\mathrm{sh}(\lambda+\eta)}, \qquad c(\lambda) = \frac{\mathrm{sh}(\eta)}{\mathrm{sh}(\lambda+\eta)}. \tag{7}$$

This is the well-known 6-vertex model solution of the Yang–Baxter equation (1). It generates the Hamiltonian of the XXZ chain with local spins $\frac{1}{2}$. $R(\lambda)$ satisfies (2)–(5) with

$$\rho(\lambda) = 1, \qquad \tilde{\rho}(\lambda) = \frac{\mathrm{sh}(\lambda)\mathrm{sh}(\lambda+2\eta)}{\mathrm{sh}^2(\lambda+\eta)}. \tag{8}$$

Every solution $R(\lambda, \mu)$ of the Yang–Baxter equation (1) determines the structure of a Yang–Baxter algebra with generators $T^{\alpha}_{\beta}(\lambda)$, $\alpha, \beta = 1, \ldots, d$, through the relations

$$R_{12}(\lambda, \mu) T_1(\lambda) T_2(\mu) = T_2(\mu) T_1(\lambda) R_{12}(\lambda, \mu), \tag{9}$$

where $T_1(\lambda) = T(\lambda) \otimes \mathrm{id}_V$, $T_2(\lambda) = \mathrm{id}_V \otimes T(\lambda)$. The matrix $T(\lambda)$ of generators is called the monodromy matrix. The map defined by

$$T^a(\lambda) = (T^{-1})^t(\lambda) \tag{10}$$

is an algebra automorphism, and Sklyanin calls it the antipode. He restricts his considerations to representations of the Yang–Baxter algebra (9) possessing the crossing symmetry

$$(T^a)^a(\lambda) = \vartheta(\lambda) T(\lambda - 2\eta). \tag{11}$$

Here $\vartheta(\lambda)$ is a complex function depending on the representation and η is the same parameter as in (4).

Sklyanin's construction of integrable systems with boundaries is based on the representations of two 'reflection algebras' $\mathcal{T}^{(-)}$ and $\mathcal{T}^{(+)}$ which, for given $R(\lambda)$ satisfying (1)–(5), are defined by the relations

$$R_{12}(\lambda-\mu)\mathcal{T}_1^{(-)}(\lambda) R_{12}(\lambda+\mu)\mathcal{T}_2^{(-)}(\mu) = \mathcal{T}_2^{(-)}(\mu) R_{12}(\lambda+\mu)\mathcal{T}_1^{(-)}(\lambda) R_{12}(\lambda-\mu), \tag{12a}$$

$$\begin{aligned} &R_{12}(-\lambda+\mu)\mathcal{T}_1^{(+)t_1}(\lambda) R_{12}(-\lambda-\mu-2\eta)\mathcal{T}_2^{(+)t_2}(\mu) \\ &\quad = \mathcal{T}_2^{(+)t_2}(\mu) R_{12}(-\lambda-\mu-2\eta)\mathcal{T}_1^{(+)t_1}(\lambda) R_{12}(-\lambda+\mu). \end{aligned} \tag{12b}$$

We shall call $\mathcal{T}^{(-)}$ and $\mathcal{T}^{(+)}$ left and right reflection algebras, respectively. $\mathcal{T}^{(-)}$ and $\mathcal{T}^{(+)}$ are isomorphic and several isomorphisms are explicitly known [17]. Using (12) and (2)–(5) Sklyanin proved the basic.

Theorem 1. *The functions ('transfer matrices')*

$$t(\lambda) = \operatorname{tr} \mathcal{T}^{(+)}(\lambda)\mathcal{T}^{(-)}(\lambda) \tag{13}$$

defined in the tensor product $\mathcal{T}^{(+)} \otimes \mathcal{T}^{(-)}$ form a commutative family, i.e.

$$[t(\lambda), t(\mu)] = 0 \quad \textit{for all } \lambda, \mu \in \mathbb{C}. \tag{14}$$

Thus, given a pair of representations of $\mathcal{T}^{(+)}$ and $\mathcal{T}^{(-)}$ the matrix $t(\lambda)$ provides a generating function of 'quantum integrals of motion'. Further following Sklyanin [17] we shall now review a set of basic results on the representation theory of $\mathcal{T}^{(+)}$ and $\mathcal{T}^{(-)}$ that will be needed in the following.

Proposition 1. *Let $\tilde{\mathcal{T}}^{(\pm)}(\lambda)$ be two representations of $\mathcal{T}^{(\pm)}$, respectively, in spaces $\tilde{W}^{\pm}$, and $T^{(\pm)}(\lambda)$ be the two representations of the Yang–Baxter algebra (9) in $W^{\pm}$ such that $T^{(+)}(\lambda)$ satisfies (11). Then*

$$\mathcal{T}^{(-)}(\lambda) = T^{(-)}(\lambda)\tilde{\mathcal{T}}^{(-)}(\lambda)T^{(-)-1}(-\lambda), \tag{15a}$$

$$\mathcal{T}^{(+)t}(\lambda) = T^{(+)t}(\lambda)\tilde{\mathcal{T}}^{(+)t}(\lambda)T^{(+)a}(-\lambda) \tag{15b}$$

are representations of $\mathcal{T}^{(\pm)}$ in $\tilde{W}^{\pm} \otimes W^{\pm}$.

Proposition 1 allows one to construct integrable open boundary conditions for known models with L-matrix $L(\lambda)$. These are connected with the simplest representations, namely c-number matrices, of $\mathcal{T}^{(\pm)}$. Given two representations $K^{(\pm)}(\lambda)$ of $\mathcal{T}^{(\pm)}$ in $\mathbb{C}$ and an L-matrix representation $L(\lambda)$ (acting on 'a local quantum space') of the Yang–Baxter algebra (9), define

$$T^{(-)}(\lambda) = L_M(\lambda) \cdots L_1(\lambda), \tag{16}$$

$$T^{(+)}(\lambda) = L_L(\lambda) \cdots L_{M+1}(\lambda), \tag{17}$$

$$\tilde{\mathcal{T}}^{(\pm)}(\lambda) = K^{(\pm)}(\lambda). \tag{18}$$

Then, by proposition 1, $\mathcal{T}^{(-)}(\lambda) = T^{(-)}(\lambda)\tilde{\mathcal{T}}^{(-)}(\lambda)T^{(-)-1}(-\lambda)$ and $\mathcal{T}^{(+)t}(\lambda) = T^{(+)t}(\lambda)\tilde{\mathcal{T}}^{(+)t}(\lambda)T^{(+)a}(-\lambda)$ are representations of $\mathcal{T}^{(\pm)}$ and, according to theorem 1, $t(\lambda) = \operatorname{tr} \mathcal{T}^{(+)}(\lambda)\mathcal{T}^{(-)}(\lambda)$ generates a commutative family of operators. Moreover, the following proposition holds.

Proposition 2. *The generating function $t(\lambda) = \operatorname{tr} \mathcal{T}^{(+)}(\lambda)\mathcal{T}^{(-)}(\lambda)$ with $\mathcal{T}^{(\pm)}(\lambda)$ defined by (15)–(18) can be written as*

$$t(\lambda) = \operatorname{tr} K^{(+)}(\lambda)T(\lambda)K^{(-)}(\lambda)T^{-1}(-\lambda), \tag{19}$$

where $T(\lambda) = T^{(+)}(\lambda)T^{(-)}(\lambda) = L_L(\lambda) \cdots L_1(\lambda)$, and is thus independent of the factorization (16), (17) of $T(\lambda)$ into $T^{(+)}(\lambda)$ and $T^{(-)}(\lambda)$.

Let us now consider any fundamental model associated with a regular R-matrix satisfying $R(0) = P$ (for a pedagogical review of such type of models see e.g. chapter 12 of [5]). Its L-matrices have matrix elements $L_{j\,\beta}^{\ \alpha}(\lambda) = R_{\beta\delta}^{\alpha\gamma}(\lambda)e_{j\,\gamma}^{\ \delta}$, $j = 1, \ldots, L$, where the e_{α}^{β} are matrices with a single non-zero entry 1 at the intersection of the αth row and the βth column, $\alpha, \beta = 1, \ldots, d$. The Hamiltonian associated with a fundamental model is

$$H = (\operatorname{tr} T(0))^{-1}\partial_{\lambda} \operatorname{tr} T(\lambda)|_{\lambda=0} = \sum_{j=1}^{L-1} H_{jj+1} + H_{L1}, \tag{20}$$

$$H_{jk} = \partial_\lambda (PR)_{jk}(\lambda)|_{\lambda=0}. \tag{21}$$

The occurrence of the term H_{L1} on the right-hand side means that we are dealing with periodic boundary conditions. Using $t(\lambda)$ defined in (19) instead of the 'row-to-row transfer matrix' $\operatorname{tr} T(\lambda)$ as a generating function, we obtain the same Hamiltonian but with different boundary terms.

Proposition 3. *Consider the generating function $t(\lambda)$ defined in proposition 2 with $T(\lambda)$ being a monodromy matrix of a fundamental model and $K^{(\pm)}(\lambda)$ being c-number representations of the right and left reflection algebras (12) satisfying*

$$\operatorname{tr} K^{(+)}(\lambda) = 1, \qquad K^{(-)}(0) = \mathrm{id}_V. \tag{22}$$

Then

$$t(\lambda) = 1 + 2\lambda\mathcal{H} + \mathcal{O}(\lambda^2), \tag{23}$$

where

$$\mathcal{H} = \sum_{j=1}^{L-1} H_{jj+1} + \frac{\partial_\lambda K_1^{(-)}(\lambda)\big|_{\lambda=0}}{2} + \operatorname{tr}_0 K_0^{(+)}(0) H_{L0} \tag{24}$$

and H_{jk} is the same as in (21).

Here the two on-site terms on the right-hand side of (24) may be interpreted as external fields acting on the boundary sites 1 and L of the chain. In particular, it may be possible that both of these terms vanish for certain choices of $K^{(\pm)}(\lambda)$ (see next example below). Then we are dealing with a chain which is cut at the link between sites L and 1, and hence has reflecting ends. Note that, unlike Sklyanin, we have assumed that $\operatorname{tr} K^{(+)}(\lambda) = 1$ for all $\lambda \in \mathbb{C}$. This is not much of a restriction since the Hamiltonian turns out to be trivial if $\operatorname{tr} K^{(+)}(\lambda)$ vanishes identically, and otherwise the trace can be replaced by 1, since the reflection equations (12) are homogeneous. With $\operatorname{tr} K^{(+)}(\lambda) = 1$ the expression (24) for the Hamiltonian looks slightly simpler, and we have $t(0) = 1$ which will become important later, when we proceed to the quantum transfer matrix formalism.

Example. Diagonal solution of the reflection equations for the XXZ chain [17]. Let

$$K(\lambda, \xi) = I_2 + \operatorname{th}(\lambda) \operatorname{cth}(\xi)\sigma^z, \tag{25}$$

where I_2 denotes the 2×2 unit matrix and $\sigma^z = e_1^1 - e_2^2$ denotes the diagonal Pauli matrix. Then, up to the multiplication with an arbitrary function,

$$K^{(-)}(\lambda) = K(\lambda, \xi^-), \qquad K^{(+)}(\lambda) = \tfrac{1}{2} K(\lambda + \eta, \xi^+) \tag{26}$$

are the unique diagonal c-number solutions of (12) with R-matrix (6). They are normalized such as to fulfil (22). Inserting (6), (7), (21) and (25), (26) into (24) we obtain

$$\begin{aligned} 2\operatorname{sh}(\eta)\mathcal{H} = {} & \sum_{j=1}^{L-1} \left[\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \operatorname{ch}(\eta)\left(\sigma_j^z \sigma_{j+1}^z - 1\right)\right] \\ & + \operatorname{sh}(\eta)\left[\operatorname{cth}(\xi^-)\sigma_1^z + \operatorname{cth}(\xi^+)\sigma_L^z\right] - \operatorname{ch}(\eta). \end{aligned} \tag{27}$$

This is the open XXZ spin-$\frac{1}{2}$ chain with anisotropy parameter $\Delta = \operatorname{ch}(\eta)$ and longitudinal local magnetic fields $h^\mp = \operatorname{sh}(\eta) \operatorname{cth}(\xi^\mp)$ acting on the left and right boundaries. Note that the boundary fields vanish for $\xi^\pm = \mathrm{i}\pi/2$.

3. Quantum transfer matrix and free energy

We recall that every solution $R(\lambda, \mu) = R(\lambda - \mu)$ of the Yang–Baxter equation (1) defines an integrable vertex model with the row-to-row transfer matrix

$$\operatorname{tr} T(\lambda) = \operatorname{tr}_0 R_{0L}(\lambda, 0) \cdots R_{01}(\lambda, 0) = \operatorname{tr} L_L(\lambda) \cdots L_1(\lambda). \tag{28}$$

If $R(\lambda)$ is regular, then $\operatorname{tr} T(\lambda)$ generates a local Hamiltonian with periodic boundary conditions via (20), (21). Hence, knowing the eigenvalues of $\operatorname{tr} T(\lambda)$ means to know the eigenvalues of the Hamiltonian (20).

The row-to-row transfer matrix (28) is not the most convenient tool, however, if one wishes to study the thermodynamic properties of the Hamiltonian (20), since, for the calculation of the partition function, all eigenvalues of H, and hence all eigenvalues of $\operatorname{tr} T(\lambda)$, are needed. Fortunately, another auxiliary vertex model can be constructed by means of the same R-matrix, whose partition function in a certain so-called Trotter limit is equal to the partition function of the Hamiltonian (20) and, asymptotically for large L, is determined by a single leading eigenvalue of the associated so-called quantum transfer matrix [18, 19].

For $j = 1, \ldots, L$ and $\beta \in \mathbb{C}$ we define the monodromy matrices

$$T_j^{\mathrm{QTM}}(\lambda) = R^{t_1}_{\bar{N}j}\left(-\frac{\beta}{N}, \lambda\right) R_{j\overline{N-1}}\left(\lambda, \frac{\beta}{N}\right) \cdots R^{t_1}_{\bar{2}j}\left(-\frac{\beta}{N}, \lambda\right) R_{j\bar{1}}\left(\lambda, \frac{\beta}{N}\right). \tag{29}$$

By slight abuse of the usual terminology we shall call them the 'quantum monodromy matrices'. They define representations of the Yang–Baxter algebra as is obvious from the defining relations (9) and their transpose with respect to space 1 (see [9] for details). It is easy to see (e.g. [9]) that

$$\lim_{N\to\infty} \operatorname{tr}_{\bar{1}\cdots\bar{N}} T_1^{\mathrm{QTM}}(0) \cdots T_L^{\mathrm{QTM}}(0) = \mathrm{e}^{-\beta H}, \tag{30}$$

which is the statistical operator associated with the Hamiltonian (20) if we identify β as the inverse temperature $1/T$. It follows that the partition function of the L-site chain with periodic boundary conditions is

$$Z_L = \lim_{N\to\infty} \operatorname{tr}_{\bar{1}\cdots\bar{N}} (\operatorname{tr} T^{\mathrm{QTM}}(0))^L = \sum_{n=0}^{\infty} \Lambda_n^L(0), \tag{31}$$

where $\Lambda_n(\lambda)$ is the nth eigenvalue of the quantum transfer matrix $\operatorname{tr} T^{\mathrm{QTM}}(\lambda)$ in the Trotter limit $N \to \infty$. By definition $\Lambda_0(\lambda)$ is the eigenvalue with largest modulus at $\lambda = 0$. It must be finitely degenerate in a vicinity of zero. For simplicity we shall assume it to be non-degenerate. In any case, the free energy per lattice site in the thermodynamic limit turns out to be [18, 19]

$$f = -T \ln \Lambda_0(0). \tag{32}$$

For many models, e.g. for the XXZ chain determined by the R-matrix (6), the leading eigenvalue of the quantum transfer matrix can be calculated for every finite Trotter number N by means of the algebraic Bethe ansatz. The corresponding solutions of the Bethe ansatz equations determine auxiliary functions which can be shown to uniquely solve certain nonlinear integral equations [5, 15, 16] containing the Trotter number N as a mere parameter. In these equations the Trotter limit is easily performed analytically, and an integral formula involving the auxiliary functions can be derived for the free energy per lattice site (32). Furthermore, it was shown in [9] that the eigenvector $|\Psi_0\rangle$ corresponding to the leading eigenvalue $\Lambda_0(\lambda)$ of the quantum transfer matrix encodes the complete information about the state of thermal equilibrium and hence about all thermal correlation functions. This led to the discovery of integral representations of correlation functions of the XXZ chain at finite temperatures [9, 10]. We shall refer to $|\Psi_0\rangle$ as the 'dominant state' of the quantum transfer matrix.

4. The surface free energy as a matrix element

The derivation of the formula (30) for the statistical operator in the previous section relies on a simple generalization of the Euler formula for the exponential function. Consider a sequence of operators $(X_N)_{N=1}^{\infty}$ on a finite dimensional vector space that converges (in some appropriate norm) to a limit X. Then

$$\lim_{N\to\infty}\left(1+\frac{X_N}{N}\right)^N = \mathrm{e}^X. \tag{33}$$

We shall call this the Trotter formula.

The Trotter formula can be combined with (23) in order to obtain the statistical operator for the Hamiltonian $\mathcal{H}$ of the open boundary system as a limit. Setting

$$X_N = N\left[t\left(-\frac{\beta}{2N}\right)-1\right] \tag{34}$$

and using (23) we find that $\lim_{N\to\infty} X_N = -\beta\mathcal{H}$ and therefore, using (33),

$$\lim_{\substack{N\to\infty\\ N\in 2\mathbb{N}}} t^{\frac{N}{2}}\left(-\frac{\beta}{N}\right) = \mathrm{e}^{-\beta\mathcal{H}}. \tag{35}$$

This observation will serve us as a starting point to express the surface free energy as a matrix element of a product of local operators.

For a pair of c-number solutions $K^{(\pm)}(\lambda)$ of the reflection equations (12) let us define an operator

$$\Pi_{\bar{k}\bar{\ell}}(\lambda) = K^{(+)}_{\bar{k}}(\lambda)P^{t_{\bar{1}}}_{\bar{k}\bar{\ell}}K^{(-)}_{\bar{k}}(\lambda), \qquad k,\ell = 1,\ldots,N. \tag{36}$$

Proposition 4. *The surface free energy, i.e. the difference between the free energies of the open system with Hamiltonian (24) and the corresponding periodically closed system with Hamiltonian (20) is given by*

$$\Delta F = \lim_{\substack{N\to\infty\\ N\in 2\mathbb{N}}} -T\ln\langle\Psi_0|\Pi_{\bar{1}\bar{2}}\left(-\frac{\beta}{N}\right)\cdots\Pi_{\overline{N-1}\bar{N}}\left(-\frac{\beta}{N}\right)|\Psi_0\rangle, \tag{37}$$

where $|\Psi_0\rangle$ *is the dominant state of the quantum transfer matrix* $\operatorname{tr} T^{\mathrm{QTM}}(\lambda)$ *(see (29)).*

Proof. Let us define

$$T_{\bar{k}}(\lambda) = R_{\bar{k}L}(\lambda,0)\cdots R_{\bar{k}1}(\lambda,0), \tag{38a}$$

$$\overline{T}_{\bar{k}}(\lambda) = R_{1\bar{k}}(0,\lambda)\cdots R_{L\bar{k}}(0,\lambda) \tag{38b}$$

for $k = 1,\ldots,N$ (remark: then $\overline{T}_{\bar{k}}(\lambda) = T^{-1}_{\bar{k}}(\lambda)$ for unitary R matrices with $\rho(\lambda) = 1$ [4]). It follows that

$$\begin{aligned} t(\lambda) &= \operatorname{tr}_{\bar{1}} K^{(+)}_{\bar{1}}(\lambda)T_{\bar{1}}(\lambda)K^{(-)}_{\bar{1}}(\lambda)\overline{T}_{\bar{1}}(-\lambda)\\ &= \operatorname{tr}_{\bar{1}\bar{2}} K^{(+)}_{\bar{1}}(\lambda)P_{\bar{1}\bar{2}}T_{\bar{1}}(\lambda)K^{(-)}_{\bar{1}}(\lambda)\overline{T}_{\bar{1}}(-\lambda)\\ &= \operatorname{tr}_{\bar{1}\bar{2}} K^{(+)}_{\bar{1}}(\lambda)(T_{\bar{2}}(\lambda)P_{\bar{1}\bar{2}})^{t_{\bar{2}}}K^{(-)}_{\bar{1}}(\lambda)\overline{T}_{\bar{1}}(-\lambda)\\ &= \operatorname{tr}_{\bar{1}\bar{2}} K^{(+)}_{\bar{1}}(\lambda)P^{t_{\bar{1}}}_{\bar{1}\bar{2}}K^{(-)}_{\bar{1}}(\lambda)T^{t}_{\bar{2}}(\lambda)\overline{T}_{\bar{1}}(-\lambda)\\ &= \operatorname{tr}_{\bar{1}\bar{2}}\Pi_{\bar{1}\bar{2}}(\lambda)T^{t}_{\bar{2}}(\lambda)\overline{T}_{\bar{1}}(-\lambda). \end{aligned} \tag{39}$$

[4] Henceforth we simply assume that $\rho(\lambda) = 1$. This can usually be achieved by properly normalizing the R-matrix and is certainly true for the R-matrix (6) of the XXZ chain (see equation (8)).

Hence,

$$t^{\frac{N}{2}}\left(-\frac{\beta}{N}\right) = \mathrm{tr}_{\bar{1}\cdots\bar{N}}\Pi_{\overline{N-1}\bar{N}}T^t_{\bar{N}}\left(-\frac{\beta}{N}\right)\overline{T}_{\overline{N-1}}\left(\frac{\beta}{N}\right)\cdots\Pi_{\bar{1}\bar{2}}T^t_{\bar{2}}\left(-\frac{\beta}{N}\right)\overline{T}_{\bar{1}}\left(\frac{\beta}{N}\right)$$
$$= \mathrm{tr}_{\bar{1}\cdots\bar{N}}\Pi_{\bar{1}\bar{2}}\Pi_{\bar{3}\bar{4}}\cdots\Pi_{\overline{N-1}\bar{N}}T^t_{\bar{N}}\left(-\frac{\beta}{N}\right)\overline{T}_{\overline{N-1}}\left(\frac{\beta}{N}\right)\cdots T^t_{\bar{2}}\left(-\frac{\beta}{N}\right)\overline{T}_{\bar{1}}\left(\frac{\beta}{N}\right)$$
$$= \mathrm{tr}_{\bar{1}\cdots\bar{N}}\Pi_{\bar{1}\bar{2}}\Pi_{\bar{3}\bar{4}}\cdots\Pi_{\overline{N-1}\bar{N}}T_1^{\mathrm{QTM}}(0)\cdots T_L^{\mathrm{QTM}}(0). \tag{40}$$

For the last line compare equation (24) of [9]. For simplicity we left out the argument $-\beta/N$ of the operators Π here. Using (35) we obtain the partition function $\mathcal{Z}_L$ of the L-site open system as

$$\mathcal{Z}_L = \lim_{\substack{N\to\infty\\ N\in 2\mathbb{N}}}\mathrm{tr}_{\bar{1}\cdots\bar{N}}\Pi_{\bar{1}\bar{2}}\left(-\frac{\beta}{N}\right)\cdots\Pi_{\overline{N-1}\bar{N}}\left(-\frac{\beta}{N}\right)(\mathrm{tr}\,T^{\mathrm{QTM}}(0))^L$$
$$= \lim_{\substack{N\to\infty\\ N\in 2\mathbb{N}}}\sum_{n=0}^{d^N-1}\langle\Psi_n|\Pi_{\bar{1}\bar{2}}\left(-\frac{\beta}{N}\right)\cdots\Pi_{\overline{N-1}\bar{N}}\left(-\frac{\beta}{N}\right)|\Psi_n\rangle\Lambda_n^L(0), \tag{41}$$

where $\langle\Psi_n|$ and $|\Psi_n\rangle$ are the left and right eigenvectors of the quantum transfer matrix. Comparing (31) and (41) we conclude that

$$\lim_{L\to\infty}\frac{\mathcal{Z}_L}{Z_L} = \langle\Psi_0|\Pi_{\bar{1}\bar{2}}\left(-\frac{\beta}{N}\right)\cdots\Pi_{\overline{N-1}\bar{N}}\left(-\frac{\beta}{N}\right)|\Psi_0\rangle \tag{42}$$

which completes the proof of proposition 4. □

Let us examine the structure of the operator Π, equation (36). Its components are

$$\Pi^{\alpha\gamma}_{\beta\delta}(\lambda) = K^{(+)}(\lambda)^\alpha_\gamma K^{(-)}(\lambda)^\delta_\beta. \tag{43}$$

This suggests to introduce row and column vectors $|-\rangle$ and $\langle+|$ with components

$${}_{\alpha\beta}|-\rangle = K^{(-)}(\lambda)^\beta_\alpha, \qquad \langle+|^{\alpha\beta} = K^{(+)}(\lambda)^\alpha_\beta. \tag{44}$$

Then

$$\Pi^{\alpha\gamma}_{\beta\delta}(\lambda) =_{\beta\delta}|-\rangle\langle+|^{\alpha\gamma} = (|-\rangle\otimes\langle+|)^{\alpha\gamma}_{\beta\delta}. \tag{45}$$

As usual we leave out the tensor product sign and write $\Pi(\lambda) = |-\rangle\langle+|$. From the definitions of $|-\rangle$ and $\langle+|$ it follows that $|-\rangle\langle+|$ is proportional to a one-dimensional projector,

$$\Pi^2(\lambda) = \langle+|-\rangle\Pi(\lambda), \qquad \langle+|-\rangle = \mathrm{tr}\,K^{(+)}(\lambda)K^{(-)}(\lambda). \tag{46}$$

Example. Let us illustrate our result with the example of the diagonal 'K-matrices' (26) of the XXZ chain. For these matrices

$$|-\rangle = \frac{1}{\mathrm{sh}(\xi^-)\mathrm{ch}(\lambda)}(\mathrm{sh}(\xi^-+\lambda),0,0,\mathrm{sh}(\xi^--\lambda)), \tag{47}$$

$$\langle+| = \frac{1}{2\mathrm{sh}(\xi^+)\mathrm{ch}(\lambda+\eta)}(\mathrm{sh}(\xi^++\lambda+\eta),0,0,\mathrm{sh}(\xi^+-\lambda-\eta))^t. \tag{48}$$

Hence,

$$\Pi(\lambda) = |-\rangle\langle+| = \frac{1}{2\mathrm{sh}(\xi^+)\mathrm{sh}(\xi^-)\mathrm{ch}(\lambda)\mathrm{ch}(\lambda+\eta)}$$
$$\times\begin{pmatrix}\mathrm{sh}(\xi^-+\lambda)\mathrm{sh}(\xi^++\lambda+\eta) & 0 & 0 & \mathrm{sh}(\xi^--\lambda)\mathrm{sh}(\xi^++\lambda+\eta)\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ \mathrm{sh}(\xi^-+\lambda)\mathrm{sh}(\xi^+-\lambda-\eta) & 0 & 0 & \mathrm{sh}(\xi^--\lambda)\mathrm{sh}(\xi^+-\lambda-\eta)\end{pmatrix} \tag{49}$$

and

$$\langle +|-\rangle = 1 + \mathrm{cth}(\xi^-)\,\mathrm{cth}(\xi^+)\,\mathrm{th}(\lambda)\,\mathrm{th}(\lambda+\eta). \tag{50}$$

As we remarked above, open boundaries with vanishing boundary fields are realized for $\xi^+ = \xi^- = \mathrm{i}\pi/2$. Then $\mathrm{sh}(\mathrm{i}\pi/2 + \lambda) = \mathrm{ich}(\lambda)$ and thus

$$\Pi(\lambda) = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}, \tag{51}$$

which is a λ-independent true projection operator.

5. The finite temperature boundary operator

In proposition 4 we have expressed the surface free energy as an expectation value of a product of certain projection operators Π in the dominant state of the quantum transfer matrix. The projectors Π are local in the space where the quantum transfer matrix acts. Having in mind that, within the algebraic Bethe ansatz, the dominant state is constructed by acting with certain creation-operator-like monodromy matrix elements on a 'Fock vacuum', we would like to express the product of projection operators in equation (37) as well in terms of elements of the monodromy matrix. This is possible by means of an inversion formula obtained in [11, 13].

Instead of working out all steps in full generality we shall stick from now on with the example of the XXZ chain. The final result will be of sufficiently general appearance, and we shall indicate how to move on to other systems. In case of the XXZ chain the auxiliary vector space V is two dimensional, and the quantum monodromy matrix (29) becomes a 2×2 matrix when expressed in terms of the L-matrices

$$\mathcal{L}_n(\lambda,\mu) = \begin{pmatrix} e_{n1}^{\,1} + b(\lambda-\mu)e_{n2}^{\,2} & c(\lambda-\mu)e_{n2}^{\,1} \\ c(\lambda-\mu)e_{n1}^{\,2} & b(\lambda-\mu)e_{n1}^{\,1} + e_{n2}^{\,2} \end{pmatrix}, \tag{52}$$

$$\tilde{\mathcal{L}}_n(\mu,\lambda) = \begin{pmatrix} e_{n1}^{\,1} + b(\mu-\lambda)e_{n2}^{\,2} & c(\mu-\lambda)e_{n1}^{\,2} \\ c(\mu-\lambda)e_{n2}^{\,1} & b(\mu-\lambda)e_{n1}^{\,1} + e_{n2}^{\,2} \end{pmatrix}, \tag{53}$$

namely,

$$T^{\mathrm{QTM}}(\lambda) = \tilde{\mathcal{L}}_N\left(-\frac{\beta}{N},\lambda\right)\mathcal{L}_{N-1}\left(\lambda,\frac{\beta}{N}\right)\cdots\tilde{\mathcal{L}}_2\left(-\frac{\beta}{N},\lambda\right)\mathcal{L}_1\left(\lambda,\frac{\beta}{N}\right). \tag{54}$$

The aforementioned inversion formula [11, 13] applies to the monodromy matrix corresponding to the usual row-to-row transfer matrix, not to the quantum monodromy matrix. Fortunately however, in case of the XXZ chain the different types of monodromy matrices are simply related by means of the crossing symmetry.

$$\frac{\tilde{\mathcal{L}}_j(\mu,\lambda)}{b(\mu-\lambda)} = \sigma_j^y\mathcal{L}_j(\lambda,\mu+\eta)\sigma_j^y, \tag{55}$$

where σ_j^y is the Pauli matrix $\sigma^y = \left(\begin{smallmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{smallmatrix}\right)$ acting on site j. Setting

$$S = \sigma_N^y\sigma_{N-2}^y\cdots\sigma_2^y, \qquad a(\lambda) = b^{\frac{N}{2}}\left(-\frac{\beta}{N}-\lambda\right), \tag{56}$$

we find that

$$\frac{T^{\mathrm{QTM}}(\lambda)}{a(\lambda)} = S\mathcal{L}_N\left(\lambda, \eta - \frac{\beta}{N}\right)\mathcal{L}_{N-1}\left(\lambda, \frac{\beta}{N}\right)\cdots\mathcal{L}_2\left(\lambda, \eta - \frac{\beta}{N}\right)\mathcal{L}_1\left(\lambda, \frac{\beta}{N}\right)S$$
$$= ST(\lambda|\xi_1, \ldots, \xi_N)S, \tag{57}$$

where $T(\lambda|\xi_1, \ldots, \xi_N) =: T(\lambda)$ is the inhomogeneous row-to-row transfer matrix with inhomogeneities

$$\xi_j = \begin{cases} \eta - \dfrac{\beta}{N} & \text{if} \quad j \text{ even} \\ \dfrac{\beta}{N} & \text{if} \quad j \text{ odd.} \end{cases} \tag{58}$$

The right-hand side of (57) admits the application of the inversion formula [11, 13]

$$e_{n\beta}^{\alpha} = \left[\prod_{j=1}^{n-1} \mathrm{tr}\, T(\xi_j)\right] T_{\beta}^{\alpha}(\xi_n) \left[\prod_{j=n+1}^{N} \mathrm{tr}\, T(\xi_j)\right]. \tag{59}$$

The left-hand side is the rescaled quantum monodromy matrix. We abbreviate it as

$$\frac{T^{\mathrm{QTM}}(\lambda)}{a(\lambda)} =: \tilde{T}^{\mathrm{QTM}}(\lambda) =: \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}. \tag{60}$$

Taking into account that

$$Se_{n\beta}^{\alpha}S = (\sigma^y)^{n+1\,\alpha}_{\ \ \gamma} e_{n\delta}^{\gamma} (\sigma^y)^{n+1\,\delta}_{\ \ \beta}, \qquad S^2 = 1 \tag{61}$$

we obtain the following inversion formula for the rescaled quantum monodromy matrix (60).

Proposition 5.

$$e_{n\beta}^{\alpha} = \left[\prod_{j=1}^{n-1} \mathrm{tr}\, \tilde{T}^{\mathrm{QTM}}(\xi_j)\right] [(\sigma^y)^{n+1} \tilde{T}^{\mathrm{QTM}}(\xi_n)(\sigma^y)^{n+1}]_{\beta}^{\alpha} \left[\prod_{j=n+1}^{N} \mathrm{tr}\, \tilde{T}^{\mathrm{QTM}}(\xi_j)\right]. \tag{62}$$

This has an immediate application to our problem of expressing the projection operator Π, equation (36), in terms of monodromy matrix elements,

$$\Pi_{2n-1\,2n}\left(-\frac{\beta}{N}\right) = \left[\prod_{j=1}^{2n-2} \mathrm{tr}\, \tilde{T}^{\mathrm{QTM}}(\xi_j)\right] \tau\left(-\frac{\beta}{N}\right) \left[\prod_{j=2n+1}^{N} \mathrm{tr}\, \tilde{T}^{\mathrm{QTM}}(\xi_j)\right], \tag{63}$$

$$\tau(\lambda) = \mathrm{tr}\, K^{(-)}(\lambda)\tilde{T}^{\mathrm{QTM}}(-\lambda)K^{(+)}(\lambda)\sigma^y \tilde{T}^{\mathrm{QTM\,t}}(\lambda + \eta)\sigma^y. \tag{64}$$

We shall call τ the 'finite temperature boundary operator'. Equation (63) implies that

$$\Pi_{12}\left(-\frac{\beta}{N}\right)\Pi_{34}\left(-\frac{\beta}{N}\right)\cdots\Pi_{N-1\,N}\left(-\frac{\beta}{N}\right) = \tau^{\frac{N}{2}}\left(-\frac{\beta}{N}\right), \tag{65}$$

where we have used (57), (60) and lemma 5 of [11]. Inserting equation (65) into (37) we can formulate the following theorem.

Theorem 2. *The surface free energy of the open XXZ chain is determined by*

$$\Delta F = \lim_{\substack{N\to\infty \\ N\in 2\mathbb{N}}} -T \ln \frac{\langle\{\lambda\}|\tau^{\frac{N}{2}}\left(-\frac{\beta}{N}\right)|\{\lambda\}\rangle}{\langle\{\lambda\}|\{\lambda\}\rangle}, \tag{66}$$

where $|\{\lambda\}\rangle$ *is the unnormalized dominant state of the rescaled quantum transfer matrix* $\operatorname{tr}\tilde{T}^{\mathrm{QTM}}(\lambda)$*, equation (60), and* τ *is the finite temperature boundary operator as defined in (64).*

Recall that within the scheme of the algebraic Bethe ansatz the vectors $|\{\lambda\}\rangle$ and $\langle\{\lambda\}|$ are given by

$$|\{\lambda\}\rangle = B(\lambda_1)\cdots B\big(\lambda_{\frac{N}{2}}\big)|0\rangle, \qquad \langle\{\lambda\}| = \langle 0|C\big(\lambda_{\frac{N}{2}}\big)\cdots C(\lambda_1), \tag{67}$$

where $B(\lambda)$ and $C(\lambda)$ have been defined in (60), where $|0\rangle = \left[\binom{1}{0}\otimes\binom{0}{1}\right]^{\otimes N/2}$ is the staggered pseudo vacuum of the quantum transfer matrix with dual $\langle 0|$, and where $\{\lambda_j\}_{j=1}^{N/2}$ is the solution of the Bethe ansatz equations

$$\left[\frac{\operatorname{sh}\big(\lambda_j+\frac{\beta}{N}\big)\operatorname{sh}\big(\lambda_j-\frac{\beta}{N}+\eta\big)}{\operatorname{sh}\big(\lambda_j-\frac{\beta}{N}\big)\operatorname{sh}\big(\lambda_j+\frac{\beta}{N}-\eta\big)}\right]^{\frac{N}{2}} = \prod_{\substack{k=1\\k\neq j}}^{N/2}\frac{\operatorname{sh}(\lambda_j-\lambda_k+\eta)}{\operatorname{sh}(\lambda_j-\lambda_k-\eta)}, \tag{68}$$

$j = 1,\ldots,N/2$, that maximizes the modulus of the leading eigenvalue of the quantum transfer matrix at $\lambda = 0$.

Example. As an example let us again consider the XXZ chain with reflecting ends, i.e. vanishing boundary fields. We have to set $\xi^{\pm} = \mathrm{i}\pi/2$ in (25), leading to $2K^{(+)}(\lambda) = K^{(-)}(\lambda) = I_2$, the 2×2 unit matrix. Inserting this into the definition (64) of the finite temperature boundary operator we obtain

$$\begin{aligned}\tau(\lambda) &= \tfrac{1}{2}\operatorname{tr}\tilde{T}^{\mathrm{QTM}}(-\lambda)\sigma^y\tilde{T}^{\mathrm{QTM\,t}}(\lambda+\eta)\sigma^y\\ &= \tfrac{1}{2}(A(-\lambda)D(\lambda+\eta) - B(-\lambda)C(\lambda+\eta) - C(-\lambda)B(\lambda+\eta) + D(-\lambda)A(\lambda+\eta)).\end{aligned} \tag{69}$$

In the remaining part of this section we would like to demonstrate that the finite temperature boundary operator $\tau(\lambda)$ is generically connected with the reflection algebra (12). Our basic result is given as follows.

Proposition 6. *With any c-number representation* $K^{(+)}(\lambda)$ *of the right reflection algebra (12b) the matrix*

$$\mathcal{T}^{(+)t}(\lambda) = \tilde{T}^{\mathrm{QTM}}(-\lambda)K^{(+)}(\lambda)\sigma^y\tilde{T}^{\mathrm{QTM\,t}}(\lambda+\eta)\sigma^y \tag{70}$$

as well defines a representation of (12b).

Proof. We only sketch the proof. The idea is to show that

$$T^{(+)}(\lambda) := \tilde{T}^{\mathrm{QTMt}}(-\lambda), \tag{71}$$

which clearly defines a representation of the Yang–Baxter algebra (9), satisfies (11), and then to employ proposition 1. In order to show that $T^{(+)}(\lambda)$ satisfies (11) one may, for instance, use (57), (60) and apply to the elementary L-matrix (52) equation (55) and the general relation

$$T^{-1}(\lambda) = \frac{\sigma^y T^t(\lambda-\eta)\sigma^y}{\det_q T(\lambda)} \tag{72}$$

for the inverse of a monodromy matrix associated with the R-matrix (6). Note that $\det_q T(\lambda)$ in (72) denotes the quantum determinant (see e.g. [17] or chapter 14 of [5]). For $T^{(+)}(\lambda)$ the function $\vartheta(\lambda)$ in (11) turns out to be

$$\vartheta(\lambda) = \left[\frac{b\big(-\lambda+\frac{\beta}{N}-\eta\big)b\big(-\lambda-\frac{\beta}{N}\big)}{b\big(-\lambda-\frac{\beta}{N}+\eta\big)b\big(-\lambda+\frac{\beta}{N}\big)}\right]^{\frac{N}{2}}. \tag{73}$$

Knowing that $T^{(+)}(\lambda)$ satisfies (11) we apply proposition 1 to the special case, when $\tilde{T}^{(+)}(\lambda) = K^{(+)}(\lambda)$ is a c-number representation of the right reflection algebra (12*b*). Then also $K^{(+)t}(\lambda)$ is a c-number representation of (12*b*), which can be seen by taking the transpose of (12*b*) and using the symmetry of the R-matrix. Taking into account that

$$T^{(+)a}(-\lambda) = \frac{\tilde{T}^{\mathrm{QTM}-1}(\lambda+2\eta)}{\vartheta(-\lambda)} = \frac{\sigma^y \tilde{T}^{\mathrm{QTM}\,t}(\lambda+\eta)\sigma^y}{\vartheta(-\lambda)\det_q \tilde{T}^{\mathrm{QTM}}(\lambda+2\eta)}, \tag{74}$$

the proposition follows. □

Proposition 6 has a number of simple but important consequences.

Corollary 1. *For any pair of c-number solutions $K^{(\pm)}(\lambda)$ of the reflection equations (12) the following holds.*

(i) The finite temperature boundary operator $\tau(\lambda)$, equation (64), defines a commuting family of operators,

$$[\tau(\lambda), \tau(\mu)] = 0 \qquad \textit{for all} \quad \lambda, \mu \in \mathbb{C}. \tag{75}$$

(ii) $\tau(\lambda)$ can be diagonalized by means of the algebraic Bethe ansatz.

(iii) The matrix element

$$\Phi\big(v_1, \ldots, v_{\frac{N}{2}}\big) = \langle\{\lambda\}| \prod_{j=1}^{N/2} \tau(v_j) |\{\lambda\}\rangle \tag{76}$$

is a symmetric function of the parameters $v_j \in \mathbb{C}$, $j = 1, \ldots, N/2$.

6. Conclusions

We have expressed the surface free energy for the XXZ chain in the thermodynamic limit as Trotter limits (37) and (66) of expectation values of certain operators in the dominant eigenstate of the quantum transfer matrix.

In (37) the operator is local and is the product of certain projection operators Π defined in (36). This formula is not only valid for the XXZ chain with reflecting ends, but was derived for a rather large class of open boundary systems, specified by a pair of c-number solutions of the reflection equations (12). If the corresponding R-matrix of 'difference form' and satisfying (2)–(5) is regular we can always associate a quantum transfer matrix with it, and the projection operators (36) are well defined.

The operator in (66) is non-local and is a simple quadratic expression in terms of the matrix elements of the rescaled quantum monodromy matrix (60). We called it the finite temperature boundary operator. In proposition 6 and corollary 1 we worked out its relation to the reflection algebra (12). We derived (66) for the case of the XXZ chain with boundary conditions specified by any c-number representation of the reflection algebra (12). Still, we used only a few rather general properties of monodromy matrices connected to the R-matrix of the XXZ chain, namely the crossing relation in the form (55) and the existence of a quantum determinant, which allowed us to apply the inversion formula (72). It seems rather likely that a finite temperature boundary operator can be defined for all solvable systems having these additional properties.

The explicit calculation of the surface free energy from our formulae remains a challenging task, since the calculation of matrix elements, such as in (37) and (66), within the algebraic Bethe ansatz is, in general, involved. In the light of the results obtained e.g. in [10, 14] there is, however, hope to accomplish this challenging task in the future.

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