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Truncation identities for the small polaron fusion hierarchy

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New Journal of Physics **15** (2013) 043026 (31pp)

Received 28 November 2012

Published 17 April 2013

Online at <http://www.njp.org/>

doi:10.1088/1367-2630/15/4/043026

Abstract. We study a one-dimensional lattice model of interacting spinless fermions. This model is integrable for both periodic and open boundary conditions; the latter case includes the presence of Grassmann valued non-diagonal boundary fields breaking the bulk $U(1)$ symmetry of the model. Starting from the embedding of this model into a graded Yang–Baxter algebra, an infinite hierarchy of commuting transfer matrices is constructed by means of a fusion procedure. For certain values of the coupling constant related to anisotropies of the underlying vertex model taken at roots of unity, this hierarchy is shown to truncate giving a finite set of functional equations for the spectrum of the transfer matrices. For generic coupling constants, the spectral problem is formulated in terms of a functional (or TQ-)equation which can be solved by Bethe ansatz methods for periodic and diagonal open boundary conditions. Possible approaches for the solution of the model with generic non-diagonal boundary fields are discussed.

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1. Introduction

The small polaron model provides an effective description of the behavior of an additional electron in a polar crystal [1, 2]. In one spatial dimension, this lattice system of interacting spinless fermions can be constructed within the framework of the quantum inverse scattering method [3] allowing us to compute the excitation spectrum by Bethe ansatz techniques, see e.g. [4, 5]. By means of a graded generalization [6–8] of Sklyanin's reflection algebra [9], it was possible to provide the small polaron model with open boundary conditions (OBC) while keeping its integrability intact. These integrable boundary conditions are encoded in c -number valued 2×2 -matrix solutions to the reflection equations [10–12].

Diagonal boundary matrices correspond to boundary chemical potentials in the Hamiltonian. In this case the small polaron model is equivalent to the spin-1/2 XXZ Heisenberg

chain with boundary magnetic fields by means of a Jordan–Wigner transformation, similarly as in the case of periodic boundary conditions (PBC) where this equivalence holds up to a boundary twist depending on the particle number [4, 13]. As a consequence, the spectrum of the open small polaron model can be obtained using Bethe ansatz methods [13–15]. For general non-diagonal solutions to the reflection equations, this equivalence does not hold as a consequence of the non-local nature of the Jordan–Wigner transformation. Furthermore, the underlying grading implies that solutions to the reflection equations for the small polaron model are *super matrices* [16]. In the corresponding Hamiltonian, the resulting additional boundary terms do not conserve particle number and have anti-commuting scalars, i.e. odd Grassmann numbers, as amplitudes. The fact that the $U(1)$ symmetry of the model is broken implies that in general there is no simple eigenstate (e.g. the Fock vacuum) of the model that can be used as a reference state for the algebraic Bethe ansatz. Therefore, alternative approaches such as functional Bethe ansatz methods have to be employed to analyze the spectrum of the model. This situation is, in fact, very similar to the case of non-diagonal boundary magnetic fields in the spin-1/2 Heisenberg chains: in the approaches used so far the solution of the spectral problem relies on constraints between the boundary fields at the two ends of the chain or restrictions on the anisotropy, or it is limited to small finite systems thereby reducing their usefulness to study this system in the thermodynamic limit [17–25].

In a previous publication [26] we have investigated the applicability of Bethe ansatz methods in the simpler case of a model of free fermions with similar open boundary conditions. We found that for a certain class of non-diagonal boundary super matrices, a unitary transformation on the auxiliary space allowed for an exact solution of the free fermion model. Furthermore, the functional equations obtained there could be easily generalized to describe the spectrum of the model for arbitrary non-diagonal boundary fields. Unfortunately, this approach cannot be applied directly to the small polaron model.

In this paper we initiate a study as to whether the nilpotency of the off-diagonal boundary parameters in a graded model allows us to bypass some of the problems arising in the case of the spin-1/2 XXZ chain with non-diagonal boundary fields. Following ideas [17, 20] developed in the context of the spin-1/2 XXZ Heisenberg chain and later generalized to the XYZ chain [27] and integrable higher spin XXZ models [28], we adapt the fusion procedure [29–31] for the transfer matrix of the quantum chain to the graded case of the small polaron model. We derive the fusion hierarchy of functional equations for a commuting family of transfer matrices for the small polaron model. Assuming the existence of a certain limit, we formulate the spectral problem of this model for periodic and general open boundary conditions in terms of functional TQ-equations. For periodic and diagonal open boundary conditions, these equations are shown to coincide with the known result obtained from using the algebraic Bethe ansatz. For special values of the interaction parameter related to roots of unity of the anisotropy parameter, we derive truncation identities for the fusion of the relevant objects, in particular the transfer matrices. Using these identities the fusion hierarchy reduces to a set of relations between finitely many quantities.

2. The small polaron as a fundamental integrable model

Some materials exhibit a strong electron–phonon coupling that considerably reduces the mobility of electrons within the conduction band. This interaction may be regarded as an increase of the electron’s effective mass, thus giving rise to quasi-particles called *polareons*.

If the electron is essentially trapped at a single lattice site, the corresponding quasi-particle is said to be a *small polaron*. In this case, electron transport occurs either by thermally activated hopping (at high temperatures) or by tunneling (at low temperatures).

In the case of PBC the N -site small polaron model is characterized by the Hamiltonian

$$H^{\text{PBC}} = \sum_{j=1}^N H_{j,j+1} \quad \text{with } H_{N,N+1} \equiv H_{N,1} \quad (2.1)$$

with a Hamiltonian density $H_{j,j+1}$ defined as

$$H_{j,j+1} = -t \left(c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1} \right) + V \left(n_{j+1} n_j + \bar{n}_{j+1} \bar{n}_j \right), \quad (2.2)$$

where c_k^\dagger and c_k label the creation, respectively annihilation, operators of spinless fermions at site k , which are subject to the anticommutation relations $[c_\ell^\dagger, c_k]_+ = \delta_{\ell k}$. Moreover, it is convenient to define number operators $n_k \equiv c_k^\dagger c_k = 1 - \bar{n}_k$. In this context, the parameters t and V may be interpreted as hopping amplitude and density–density interaction strength, respectively.

2.1. Construction within the quantum inverse scattering method framework

The small polaron model can be associated with a graded six-vertex model with anisotropy η and R -matrix

$$R(u) = \frac{1}{\sin(2\eta)} \begin{pmatrix} \sin(u+2\eta) & 0 & 0 & 0 \\ 0 & \sin(u) & \sin(2\eta) & 0 \\ 0 & \sin(2\eta) & \sin(u) & 0 \\ 0 & 0 & 0 & -\sin(u+2\eta) \end{pmatrix}. \quad (2.3)$$

$R(u)$ is a solution to the Yang–Baxter equation (YBE)

$$R_{12}(u-v) R_{13}(u) R_{23}(v) = R_{23}(v) R_{13}(u) R_{12}(u-v) \quad (2.4)$$

and enjoys several useful properties, such as

- *P-symmetry*

$$R_{21}(u) \equiv \mathcal{P}_{12} R_{12}(u) \mathcal{P}_{12} = R_{12}(u), \quad (2.5a)$$

- *T-symmetry*

$$R_{12}^{\text{st}_1 \text{st}_2}(u) = R_{12}^{\text{ist}_1 \text{ist}_2}(u) = R_{21}(u), \quad (2.5b)$$

- *regularity*

$$R_{12}(0) = \mathcal{P}_{12}, \quad (2.5c)$$

- *unitarity*

$$R_{12}(u) R_{21}(-u) = \zeta(u), \quad (2.5d)$$

where the scalar function $\zeta(u)$ is given by

$$\zeta(u) \equiv g(u)g(-u) \quad \text{and} \quad g(u) \equiv -\frac{\sin(u-2\eta)}{\sin(2\eta)}.$$

Unitarity of an R -matrix is, of course, a direct consequence of its regularity.

- *Crossing symmetry*

$$R_{21}^{\text{st}_2}(-u - 4\eta) R_{21}^{\text{st}_1}(u) = \zeta(u + 2\eta), \quad (2.5e)$$

- *periodicity*

$$R_{12}(u + \pi) = -\sigma_2^z R_{12}(u) \sigma_2^z = -\sigma_1^z R_{12}(u) \sigma_1^z. \quad (2.5f)$$

The periodicity $R(u + 2\pi) = R(u)$ is obvious from definition (2.3).

The operations of partial super transposition st_a and inverse partial super transposition ist_a as well as the graded permutation operator \mathcal{P}_{ab} and the notion of super tensor product structures are explained in appendix A. Unless stated otherwise, all embeddings are to be understood in a *graded* sense, that is into a super tensor product structure. Considering the Yang–Baxter algebra (YBA)

$$R_{12}(u - v) T_1(u) T_2(v) = T_2(v) T_1(u) R_{12}(u - v), \quad (2.6)$$

this means that $T_1(u) \equiv T(u) \otimes_s \mathbb{1}$ and $T_2(v) \equiv \mathbb{1} \otimes_s T(v)$.

The small polaron model constructed here is fundamental, i.e. the Lax-operators $L_j(u)$, being local solutions to (2.6), are just graded embeddings of the above R -matrix (2.3),

$$L_j(u) = \frac{1}{\sin(2\eta)} \begin{pmatrix} \sin(u)n_j + \sin(u + 2\eta)\bar{n}_j & \sin(2\eta)c_j^\dagger \\ \sin(2\eta)c_j & \sin(u)\bar{n}_j - \sin(u + 2\eta)n_j \end{pmatrix}. \quad (2.7)$$

As a consequence of YBA's co-multiplication property, a specific global representation, the so-called monodromy matrix, can be constructed as a product of Lax-operators taken in auxiliary space,

$$T(u) \equiv L_N(u) \cdot \dots \cdot L_2(u) \cdot L_1(u), \quad (2.8)$$

and gives rise to a family of commuting (super) transfer matrices

$$\tau(u) \equiv \text{str} \{ T(u) \} \Rightarrow [\tau(u), \tau(v)] = 0 \quad \forall u, v \in \mathbb{C}, \quad (2.9)$$

where $\text{str} \{ \cdot \}$ denotes the supertrace defined in appendix A. In particular, the PBC Hamiltonian (2.1) with $t = 1$ and $V = -\cos(2\eta)$ is among these commuting operators,

$$H^{\text{PBC}} = -\sin(2\eta) \left. \frac{d}{du} \ln \tau(u) \right|_{u=0}. \quad (2.10)$$

2.2. Asymptotic behavior of the periodic boundary conditions (PBC) transfer matrix

By construction the monodromy matrix (and similarly the transfer matrix) is a Laurent polynomial in $z \equiv e^{iu}$, i.e. $T(u) = \sum_{k=-N}^N T_k z^k$. For $z \rightarrow \infty$ the Lax-operators (2.7) are

$$L_j(u) \approx \frac{z}{2i \sin(2\eta)} \begin{pmatrix} n_j + e^{2i\eta} \bar{n}_j & 0 \\ 0 & \bar{n}_j - e^{2i\eta} n_j \end{pmatrix} \quad (2.11)$$

and consequently the asymptotic behavior of the (super) transfer matrix is given by

$$\tau(u) \approx \left(\frac{z}{2i \sin(2\eta)} \right)^N e^{iN\eta} \left[\prod_{j=1}^N \left(e^{-i\eta} n_j + e^{i\eta} \bar{n}_j \right) - \prod_{j=1}^N \left(e^{-i\eta} \bar{n}_j - e^{i\eta} n_j \right) \right]. \quad (2.12)$$

As the leading term comprises only diagonal operators, the first-order contributions to the transfer matrix eigenvalues $\Lambda_M(u)$ can easily be determined and are found to depend on the total number of particles M ,

$$\Lambda_M(u) \approx e^{iuN} \left(\frac{e^{i\eta}}{e^{i2\eta} - e^{-i2\eta}} \right)^N (e^{iN\eta} e^{-iM2\eta} - (-1)^M e^{-iN\eta} e^{iM2\eta}). \quad (2.13)$$

This result will be used to fix the degree of the Q -functions in section 4.

3. Fusion of the R -matrix in auxiliary space

Given an R -matrix as a solution to the YBE (2.4), the fusion procedure [29–31] allows for the construction of *larger* R -matrices as solutions to the corresponding YBEs, where larger refers to the dimensionality of the auxiliary space involved. All that fusion requires is a pair of complementary orthogonal² projectors P_{12}^+ and P_{12}^- such that for a specific value of $\rho \in \mathbb{C}$ the following *triangularity condition* holds for arbitrary spectral parameters $u \in \mathbb{C}$:

$$P_{12}^- R_{13}(u) R_{23}(u + \rho) P_{12}^+ = 0. \quad (3.1)$$

By virtue of this condition, it can be shown that the *fused* R -matrix, defined by

$$R_{(12)3}(u) \equiv P_{12}^+ R_{13}(u) R_{23}(u + \rho) P_{12}^+, \quad (3.2)$$

satisfies the corresponding YBE

$$R_{(12)3}(u - v) R_{(12)4}(u) R_{34}(v) = R_{34}(v) R_{(12)4}(u) R_{(12)3}(u - v). \quad (3.3)$$

It is easily found that the small polaron R -matrix (2.3) has two distinct singularities at $u = \pm 2\eta$,

$$\det\{R(u)\} = -\frac{\sin(u - 2\eta)}{\sin(2\eta)} \left(\frac{\sin(u + 2\eta)}{\sin(2\eta)} \right)^3 \stackrel{!}{=} 0. \quad (3.4)$$

At $u = -2\eta$ the R -matrix gives rise to a projector onto a one-dimensional subspace,

$$P^- \equiv -\frac{1}{2} R(-2\eta) = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (3.5)$$

However, unlike in the case of the Heisenberg spin chain, the orthogonal projector P^+ onto the complementary three-dimensional subspace cannot be obtained from the R -matrix at the second singularity,

$$P^+ \equiv \mathbb{1} - P^- \neq \frac{1}{2} R(2\eta). \quad (3.6)$$

Using this projector, fusion of two small polaron R -matrices in the auxiliary space can be achieved by means of (3.2) with $\rho = 2\eta$,

$$R_{(12)3}(u) \equiv P_{12}^+ R_{13}(u) R_{23}(u + 2\eta) P_{12}^+. \quad (3.7)$$

² As usual, *orthogonal* means $P_{12}^+ P_{12}^- = 0$ whereas *complementary* refers to the property $P_{12}^+ + P_{12}^- = \mathbb{1}$.

The resulting object $R_{(12)3}(u)$ is an 8×8 -matrix of rank 6 and may therefore be effectively reduced to a 6×6 -matrix $R_{\ll 12 \gg 3}(u)$ acting on a three-dimensional auxiliary space $V_{\ll 12 \gg}$ and on a two-dimensional quantum space V_3 . Changing from the $BFFB$ -graded³ canonical basis

$$\mathcal{B}_0 = \{e_1, e_2, e_3, e_4\}_{BFFB} \equiv \{|0\rangle \otimes |0\rangle, |0\rangle \otimes |1\rangle, |1\rangle \otimes |0\rangle, |1\rangle \otimes |1\rangle\}_{BFFB} \quad (3.8)$$

to the projectors' $BFFB$ -graded singlet/triplet eigenbasis

$$\mathcal{B}_{\pm} = \{f_1, f_2, f_3, f_4\}_{BFFB} \equiv \left\{ e_1, \frac{e_2 + e_3}{\sqrt{2}}, e_4, \frac{e_2 - e_3}{\sqrt{2}} \right\}_{BFFB}, \quad (3.9)$$

the matrix $R_{(12)3}(u)$ gains the advantageous shape

$$\left(\begin{array}{c|cc} R_{\ll 12 \gg 3}(u) & & \\ \hline & 0 & 0 \\ & 0 & 0 \end{array} \right)_j^i = (f_i)^T [R_{(12)3}(u)] f_j, \quad (3.10)$$

where $R_{\ll 12 \gg 3}(u)$ is the only non-vanishing block. Explicitly, one finds

$$R_{\ll 12 \gg 3}(u) \propto \left(\begin{array}{cc|cc|cc} 2 \sin(u+4\eta) & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 \sin(u) & \sqrt{2} \sin(4\eta) & 0 & 0 & 0 \\ \hline 0 & 2\sqrt{2} \sin(2\eta) & 2 \sin(u+2\eta) & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 \sin(u+2\eta) & -2\sqrt{2} \sin(2\eta) & 0 \\ \hline 0 & 0 & 0 & \sqrt{2} \sin(4\eta) & 2 \sin(u) & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \sin(u+4\eta) \end{array} \right). \quad (3.11)$$

3.1. General construction of higher fused R -matrices

In general, higher fused R -matrices can be constructed employing the projection operators

$$P_{1\dots n}^+ \equiv \frac{1}{n!} \sum_{\sigma \in \mathcal{S}_n} P_{\sigma}. \quad (3.12)$$

Here σ runs through all the elements of the permutation group \mathcal{S}_n and P_{σ} is the permutation operator corresponding to σ . Now the higher fused R -matrices are obtained as

$$R_{(1\dots n)q}(u) \equiv P_{1\dots n}^+ R_{1q}(u) R_{2q}(u+2\eta) \dots R_{nq}(u+[n-1] \cdot 2\eta) P_{1\dots n}^+. \quad (3.13)$$

Just as for the first fusion step, it is convenient to apply a similarity transformation $A_{(1\dots n)}$ into the eigenbasis⁴ of the projection operators,

$$A_{(1\dots n)} R_{(1\dots n)q}(u) A_{(1\dots n)}^{-1} \equiv \left(\begin{array}{c|cc} R_{\ll 1\dots n \gg q}(u) & & \\ \hline & 0 & \\ & & \ddots \end{array} \right). \quad (3.14)$$

The first few ($n = 1, 2, 3, 4$) transformation matrices $A_{(1\dots n)}$ are explicitly given in appendix E. By construction, all matrix elements of (3.14), except for those in the upper left $2(n+1) \times 2(n+1)$ block, vanish. This block is referred to as the fused R -matrix $R_{\ll 1\dots n \gg q}(u)$. As shown in table 1, its fused auxiliary space has alternating gradation (bosonic, fermionic, etc).

³ This notation is explained in appendix A.

⁴ Since the projectors here are just the same as for the XXZ Heisenberg spin chain, the respective transformation is simply given by the matrix of Clebsch–Gordan coefficients.

Table 1. Gradation of the fused auxiliary spaces in the projector eigenbasis.

Auxiliary space:	$\ll 12 \gg$	$\ll 123 \gg$	$\ll 1234 \gg$	$\ll 12345 \gg$...
Grading:	BFB	$BFBF$	$BFBFB$	$BFBFBF$...

The periodicity property (2.5f) carries over to the fused R -matrices,

$$R_{\ll 1\dots n \gg q}(u + \pi) = (-1)^n \sigma_{\ll n \gg}^z R_{\ll 1\dots n \gg q}(u) \sigma_{\ll n \gg}^z \quad (3.15)$$

with $\sigma_{\ll n \gg}^z$ being defined through

$$\sigma_{(n)}^z \equiv \prod_{k=1}^n \sigma_k^z \quad \text{and} \quad A_{(12\dots n)} \sigma_{(n)}^z A_{(12\dots n)}^{-1} \equiv \left(\begin{array}{c|ccc} \sigma_{\ll n \gg}^z & & & \\ \hline & * & & \\ & & \ddots & \end{array} \right). \quad (3.16)$$

3.2. Fusion hierarchy for super transfer matrices

Since, by construction, the fused R -matrices again satisfy the YBE, they can be used to establish further families of commuting operators as supertraces of fused monodromy matrices,

$$\begin{aligned} T_{(12\dots n)}(u) &\equiv P_{12\dots n}^+ R_{(12\dots n)q_N}(u) \cdots R_{(12\dots n)q_2}(u) R_{(12\dots n)q_1}(u) P_{12\dots n}^+ \\ &= P_{12\dots n}^+ T_{(12\dots n-1)}(u) T_n(u + [n-1] \cdot 2\eta) P_{12\dots n}^+, \end{aligned} \quad (3.17)$$

$$A_{(12\dots n)} T_{(12\dots n)}(u) A_{(12\dots n)}^{-1} \equiv \left(\begin{array}{c|ccc} T_{\ll 12\dots n \gg}(u) & & c & \\ \hline & & 0 & \\ & & & \ddots \end{array} \right). \quad (3.18)$$

Indeed, it is found that the (super) transfer matrices obtained from any fusion level n ,

$$\tau^{(n)}(u) \equiv \text{str}_{(12\dots n+1)} \{ T_{(12\dots n+1)}(u) \} = \text{str}_{\ll 12\dots n+1 \gg} \{ T_{\ll 12\dots n+1 \gg}(u) \}, \quad (3.19)$$

commute with the transfer matrices of any other fusion level m , i.e. $[\tau^{(n)}(u), \tau^{(m)}(v)] = 0$ for all $u, v \in \mathbb{C}$ and arbitrary $n, m \in \mathbb{N}_0$. A most interesting fact is that these *fused* transfer matrices obey certain functional relations, known as *fusion hierarchy*. For the periodic boundary case, the fusion hierarchy reads

$$\tau^{(n)}(u) \tau^{(0)}(u + [n+1] \cdot 2\eta) = \tau^{(n+1)}(u) + \delta(u + n \cdot 2\eta) \tau^{(n-1)}(u), \quad (3.20)$$

where $\delta(u) \equiv \delta\{T(u)\}$ labels the PBC super quantum determinant (SQD) defined in appendix D. In contrast to ungraded models, such as the XXZ Heisenberg spin chain, this quantum determinant is *not* proportional to the identity.

4. TQ-equations for PBC

After applying a shift $u \rightarrow u - [n+1] \cdot 2\eta$, the PBC fusion hierarchy (3.20) reads

$$\tau^{(n)}(u - [n+1] \cdot 2\eta) \tau^{(0)}(u) = \tau^{(n+1)}(u - [n+1] \cdot 2\eta) + \delta(u - 2\eta) \tau^{(n-1)}(u - [n+1] \cdot 2\eta). \quad (4.1)$$

As all operators in this equation mutually commute, it may equally well be read as an equation for the eigenvalues $\Lambda^{(n)}(u)$ of the fused super transfer matrices. With $\Lambda(u) \equiv \Lambda^{(0)}(u)$ this yields

$$\Lambda(u) = \frac{\Lambda^{(n+1)}(u - [n+1] \cdot 2\eta)}{\Lambda^{(n)}(u - [n+1] \cdot 2\eta)} - (-1)^{N+M} \zeta^N(u) \frac{\Lambda^{(n-1)}(u - [n+1] \cdot 2\eta)}{\Lambda^{(n)}(u - [n+1] \cdot 2\eta)}, \quad (4.2)$$

where M is the number of particles in the system, such that the sign $(-1)^M$ depends on the parity of the corresponding eigenstate (bosonic/fermionic). This peculiarity stems from the fact that the PBC SQD (D.21a) cannot simply be treated as a scalar function but rather as an operator that intersperses sign factors into the respective sectors. This may be illustrated by considering the fusion hierarchy (4.1) in a diagonal basis for chain length $N = 1$,

$$\begin{pmatrix} * & \\ & * \end{pmatrix} \begin{pmatrix} * & \\ & * \end{pmatrix} = \begin{pmatrix} * & \\ & * \end{pmatrix} + \begin{pmatrix} + & \\ & - \end{pmatrix} \begin{pmatrix} * & \\ & * \end{pmatrix} \quad \begin{array}{l} \leftarrow B \\ \leftarrow F. \end{array} \quad (4.3)$$

Introducing the functions

$$\bar{Q}^{(n)}(u) \equiv \Lambda^{(n)}(u - [n+1] \cdot 2\eta), \quad (4.4)$$

the eigenvalues can be rewritten as

$$\Lambda(u) = \frac{\bar{Q}^{(n+1)}(u+2\eta)}{\bar{Q}^{(n)}(u)} - (-1)^{N+M} \zeta^N(u) \frac{\bar{Q}^{(n-1)}(u-2\eta)}{\bar{Q}^{(n)}(u)}. \quad (4.5)$$

Now factorize $\bar{Q}^{(n)}$ according to

$$\bar{Q}^{(n)} = \chi_M(u) \Upsilon_n^N(u) \cdot Q^{(n)}(u), \quad (4.6)$$

where

$$\chi_M(u) \equiv e^{i\pi(M+1)\frac{u}{2\eta}} \quad \text{and} \quad \Upsilon_n(u) \equiv \prod_{k=0}^n \frac{\sin(u - [n-k+1] \cdot 2\eta)}{\sin(2\eta)}. \quad (4.7)$$

Assuming the existence of the limit $Q(u) \equiv \lim_{n \rightarrow \infty} Q^{(n)}(u)$, this yields

$$\Lambda(u) = \left(\frac{\sin(u+2\eta)}{\sin(2\eta)} \right)^N \frac{Q(u-2\eta)}{Q(u)} - (-1)^M \left(\frac{\sin(u)}{\sin(2\eta)} \right)^N \frac{Q(u+2\eta)}{Q(u)}. \quad (4.8)$$

Due to the structure of the entries in the Lax-operators, the Q -functions as factorize as

$$Q(u) = \prod_{\ell=1}^G \sin(u - \lambda_\ell), \quad (4.9)$$

where the integer G can be determined by considering the asymptotic behavior of $\Lambda(u)$. In the limit $z \equiv e^{iu} \rightarrow \infty$, the leading contribution to (4.8) is

$$\Lambda(u) \approx e^{iNu} \left(\frac{e^{i\eta}}{e^{i2\eta} - e^{-i2\eta}} \right)^N [e^{iN\eta} e^{-iG2\eta} - (-1)^M e^{-iN\eta} e^{iG2\eta}] \quad (4.10)$$

such that consistency with (2.13) immediately fixes $G = M$. The requirement for the eigenvalues $\Lambda(u)$ to be analytic ultimately yields

$$\text{Res}_{\lambda_j}(\Lambda) = 0 \quad \Leftrightarrow \quad \left(\frac{\sin(\lambda_j + 2\eta)}{\sin(\lambda_j)} \right)^N = \prod_{\ell=1}^M \frac{\sin(\lambda_j - \lambda_\ell + 2\eta)}{\sin(\lambda_\ell - \lambda_j + 2\eta)}, \quad (4.11)$$

which are precisely the Bethe equations for this model [4, 5, 13]. Compared to the periodic XXZ Heisenberg chain, these Bethe equations exhibit an additional sign, reflecting the different twist in the boundary conditions appearing in the sectors with even and odd particle numbers through the Jordan–Wigner transformation from the fermionic to the spin model.

5. Truncation of the PBC fusion hierarchy

In the case of the XXZ-model it has been observed that for certain values of the anisotropy η the fusion hierarchy repeats itself after a finite number of steps. The small polaron model shares this feature at values $\eta = \eta_p$ where

$$\eta_p \equiv \frac{\pi/2}{p+1}. \quad (5.1)$$

5.1. R -matrix truncation

The truncation identities for the R -matrices are found to be

$$\mathcal{R}_q^{(p)}(u, \eta_p) = \begin{pmatrix} -\mathcal{M}_p(u) \sigma_q^z & & \\ & \zeta(u) \sigma_q^z \mathcal{R}_q^{(p-2)}(u + 2\eta_p, \eta_p) & \\ & & \mathcal{M}_p(u) (\sigma_q^z)^p \end{pmatrix}, \quad (5.2)$$

where

$$\begin{aligned} \mathcal{R}_q^{(p)}(u, \eta) &\equiv B_{\ll 1 \dots (p+1) \gg} R_{\ll 1 \dots (p+1) \gg q}(u) B_{\ll 1 \dots (p+1) \gg}^{-1}, \\ \mathcal{M}_p(u) &\equiv \left(\frac{1/2}{\sin(2\eta_p)} \right)^p \frac{\sin([p+1]u)}{\sin(2\eta_p)} \end{aligned} \quad (5.3)$$

with the transformation matrices $B_{\ll 1 \dots n \gg}$ explicitly given in appendix E up to $n = 4$.

5.2. Super transfer matrix truncation

For PBC the B -transformed fused monodromy matrix $\mathcal{T}^{(p)}(u, \eta)$ of an N -site model with quantum space $\mathcal{H} = V_{q_1} \otimes_s V_{q_2} \otimes_s \dots \otimes_s V_{q_N}$ is defined as

$$\begin{aligned} \mathcal{T}^{(p)}(u, \eta) &\equiv \mathcal{R}_{q_N}^{(p)}(u, \eta) \mathcal{R}_{q_{N-1}}^{(p)}(u, \eta) \dots \mathcal{R}_{q_1}^{(p)}(u, \eta) \\ &= B_{\ll 1 \dots (p+1) \gg} R_{\ll 1 \dots (p+1) \gg q_N}(u) \dots R_{\ll 1 \dots (p+1) \gg q_1}(u) B_{\ll 1 \dots (p+1) \gg}^{-1} \\ &= B_{\ll 1 \dots (p+1) \gg} T_{\ll 1 \dots (p+1) \gg}(u) B_{\ll 1 \dots (p+1) \gg}^{-1} \end{aligned} \quad (5.4)$$

and due to the cyclic invariance of the supertrace it yields the exact same transfer matrix

$$\tau^{(p)}(u, \eta) \equiv \text{str}_{\ll 1 \dots (p+1) \gg} \left\{ T_{\ll 1 \dots (p+1) \gg}(u) \right\} = \text{str}_{\ll 1 \dots (p+1) \gg} \left\{ \mathcal{T}^{(p)}(u, \eta) \right\}. \quad (5.5)$$

At $\eta = \eta_p$ the truncation identity (5.2) for R -matrices gives

$$\mathcal{T}^{(p)}(u, \eta_p) = \begin{pmatrix} [-\mathcal{M}_p(u)]^N \prod_{i=N}^1 \sigma_{q_i}^z & \\ & \zeta^N(u) \prod_{i=N}^1 \sigma_{q_i}^z \mathcal{R}_{q_i}^{(p-2)}(u+2\eta_p, \eta_p) \\ & & [\mathcal{M}_p(u)]^N \prod_{i=N}^1 (\sigma_{q_i}^z)^p \end{pmatrix} \quad (5.6)$$

such that the truncation identity for the transfer matrices is found to be

$$\begin{aligned} \tau^{(p)}(u, \eta_p) &= [-\mathcal{M}_p(u)]^N \left(\prod_{i=1}^N \sigma_{q_i}^z \right) - (-1)^p [\mathcal{M}_p(u)]^N \left(\prod_{i=1}^N (\sigma_{q_i}^z)^p \right) \\ &\quad - \zeta^N(u) \left(\prod_{i=1}^N \sigma_{q_i}^z \right) \tau^{(p-2)}(u+2\eta_p, \eta_p). \end{aligned} \quad (5.7)$$

6. The small polaron with open boundary conditions (OBC)

6.1. Reflection algebras and boundary matrices

The construction of integrable systems with open boundary conditions is based on representations of the graded reflection algebra

$$R_{12}(u-v) \mathcal{T}_1^-(u) R_{21}(u+v) \mathcal{T}_2^-(v) = \mathcal{T}_2^-(v) R_{12}(u+v) \mathcal{T}_1^-(u) R_{21}(u-v) \quad (6.1)$$

and the corresponding dual-graded reflection algebra

$$\bar{R}_{12}(v-u) \mathcal{T}_1^+(u)^{\text{st}_1} R_{21}(-u-v-4\eta) \mathcal{T}_2^+(v)^{\text{ist}_2} = \mathcal{T}_2^+(v)^{\text{ist}_2} R_{12}(-u-v-4\eta) \mathcal{T}_1^+(u)^{\text{st}_1} \bar{R}_{21}(v-u). \quad (6.2)$$

The relation between $R_{ab}(u)$ and the *conjugated* R -matrix $\bar{R}_{ab}(u)$ is explained in appendix B. c -number valued boundary matrices, compatible with the respective reflection equation, are found to be [10–12] (see also [32] for the ungraded case of the XXZ chain)

$$\begin{aligned} K^-(u) &= \omega^- \begin{pmatrix} \sin(u+\psi_-) & \alpha_- \sin(2u) \\ \beta_- \sin(2u) & -\sin(u-\psi_-) \end{pmatrix}, \\ K^+(u) &= \omega^+ \begin{pmatrix} \sin(u+2\eta+\psi_+) & \alpha_+ \sin(2[u+2\eta]) \\ \beta_+ \sin(2[u+2\eta]) & \sin(u+2\eta-\psi_+) \end{pmatrix} \end{aligned} \quad (6.3)$$

with normalizations $\omega^\pm \equiv \omega^\pm(\eta)$ defined by

$$\omega^-(\eta) \equiv \frac{1}{\sin(\psi_-)} \quad \text{and} \quad \omega^+(\eta) \equiv \frac{1}{2 \cos(2\eta) \sin(\psi_+)}. \quad (6.4)$$

These matrices share the periodicity property of the R -matrix, i.e.

$$K^\mp(u+\pi) = -\sigma^z K^\mp(u) \sigma^z. \quad (6.5)$$

Here the normalizations were chosen such that

$$K^-(0) = \mathbb{1} \quad \text{and} \quad \text{str} \{ K^+(0) \} = 1, \quad (6.6)$$

but apart from this, the two solutions are related via

$$K^+(u) = \left[\frac{1}{2 \cos(2\eta)} K^-(-u - 2\eta) \sigma^z \right]_{(\ominus \rightarrow \oplus)}, \quad (6.7)$$

where $(\ominus \rightarrow \oplus)$ marks the replacements $(\alpha_-, \beta_-, \psi_-) \rightarrow (-\alpha_+, \beta_+, -\psi_+)$. In principle, the parameters ψ_{\pm} are arbitrary even Grassmann numbers but their invertability requires them to have a non-vanishing complex part⁵. The remaining parameters α_{\pm} and β_{\pm} are odd Grassmann numbers, being subject to the condition $\alpha_{\pm}\beta_{\pm} = 0$.

Given the monodromy matrix $T(u) = L_N(u)L_{N-1}(u) \dots L_1(u)$, it is possible to construct a further representation of the reflection algebra (6.1) as

$$\mathcal{T}^-(u) = T(u) K^-(u) \widehat{T}(u) \equiv \begin{pmatrix} \mathcal{A}(u) & \mathcal{B}(u) \\ \mathcal{C}(u) & \mathcal{D}(u) \end{pmatrix}, \quad (6.8)$$

with $\widehat{T}(u)$ being a shorthand notation for $T^{-1}(-u)$,

$$\begin{aligned} \widehat{T}(u) &\equiv R_{01}^{-1}(-u) R_{02}^{-1}(-u) \dots R_{0N}^{-1}(-u) \\ &\stackrel{(2.5d)}{\equiv} \frac{1}{\zeta^N(u)} R_{10}(u) R_{20}(u) \dots R_{N0}(u) \\ &\stackrel{(2.5a)}{\equiv} \left(\frac{1}{\zeta(u)} \right)^N R_{01}(u) R_{02}(u) \dots R_{0N}(u), \end{aligned} \quad (6.9)$$

resulting in an OBC super transfer matrix

$$\tau(u) \equiv \text{str}_0 \{ K^+(u) \mathcal{T}^-(u) \}. \quad (6.10)$$

Expanding $\tau(u)$ around $u = 0$, one obtains a Hamiltonian featuring the same bulk part (2.2) as the corresponding PBC Hamiltonian. Defining the shorthand $\mathcal{N}_{\pm} \equiv \frac{1}{2} \csc(2\eta) \csc(\psi_{\pm}) \sin(2\eta \pm \psi_{\pm})$, the resulting OBC Hamiltonian

$$\begin{aligned} H^{\text{OBC}} &= \sum_{j=1}^{N-1} H_{j,j+1} + \frac{1}{2} \cot(\psi_-) [\bar{n}_1 - n_1] + [\mathcal{N}_+ \bar{n}_N - \mathcal{N}_- n_N] \\ &\quad + \csc(\psi_-) [\alpha_- c_1 - \beta_- c_1^{\dagger}] + \csc(\psi_+) [\alpha_+ c_N - \beta_+ c_N^{\dagger}] \end{aligned} \quad (6.11)$$

is derived from the set of open boundary transfer matrices by

$$\partial_u \tau(u)|_{u=0} = 2 H^{\text{OBC}} + \text{const.} \quad (6.12)$$

In the case of diagonal boundaries, i.e. $\alpha_{\pm} = \beta_{\pm} = 0$, Bethe equations can be derived using the algebraic Bethe ansatz. This allows for the computation of the transfer matrix eigenvalues and eigenvectors (see appendix C respectively [13]). Here the eigenvalues coincide with those of the spin-1/2 XXZ Heisenberg chain subject to (diagonal) boundary magnetic fields.

⁵ Such an additive part, that contains no nilpotent generators, is sometimes called the *body* of a Grassmann number. It is to be distinguished from the *soul* of a Grassmann number, which contains only sums of products of nilpotent generators.

6.2. Properties of the OBC transfer matrix

As a consequence of the properties (2.5e), (2.5f) of the R -matrix and (6.5), (6.7) of the boundary matrices, the transfer matrix (6.10) of the small polaron model enjoys several useful properties, such as

- π -periodicity

$$\tau(u + \pi) = \tau(u), \quad (6.13a)$$

- crossing symmetry

$$\zeta^N(u) \tau(u) = \zeta^N(-u - 2\eta) \tau(-u - 2\eta). \quad (6.13b)$$

In addition, $\tau(u)$ is normalized as

$$\tau(0) = \mathbb{1} \quad (6.14)$$

and becomes diagonal in the semi-classical limit $\eta \rightarrow 0$:

$$\tau(u)|_{\eta=0} = \frac{(-1)^N}{\sin(\psi_-) \sin(\psi_+)} \left(2 \sin^2(u) \cos^2(u) (\beta_+ \alpha_- - \alpha_+ \beta_-) \sigma_{(N)}^z - [\cos^2(u) \sin(\psi_-) \sin(\psi_+) + \sin^2(u) \cos(\psi_-) \cos(\psi_+)] \cdot \mathbb{1} \right). \quad (6.15)$$

The asymptotic behavior of the (super) transfer matrix in the limit $z \equiv e^{iu} \rightarrow \infty$ can be read off from its construction: that of the Lax operators $L_j(u)$ is given in equation (2.11). Similarly, we find

$$L_j^{-1}(-u) = \frac{4 \sin(2\eta)}{2i z} \begin{pmatrix} n_j + e^{2i\eta} \bar{n}_j & 0 \\ 0 & \bar{n}_j - e^{2i\eta} n_j \end{pmatrix} + \mathcal{O}\left(\frac{1}{z^2}\right), \quad (6.16a)$$

$$K^-(u) = \frac{\omega^-}{2i} \left[z^2 \begin{pmatrix} 0 & \alpha_- \\ \beta_- & 0 \end{pmatrix} + z \begin{pmatrix} e^{i\psi_-} & 0 \\ 0 & -e^{-i\psi_-} \end{pmatrix} + \mathcal{O}\left(\frac{1}{z}\right) \right], \quad (6.16b)$$

$$K^+(u) = \frac{\omega^+ e^{2i\eta}}{2i} \left[z^2 e^{2i\eta} \begin{pmatrix} 0 & \alpha_+ \\ \beta_+ & 0 \end{pmatrix} + z \begin{pmatrix} e^{i\psi_+} & 0 \\ 0 & e^{-i\psi_+} \end{pmatrix} + \mathcal{O}\left(\frac{1}{z}\right) \right]. \quad (6.16c)$$

As a consequence, the asymptotics of the OBC transfer matrix (6.10) and of their eigenvalues is given by

$$\tau(u) = (-1)^N \frac{\omega^+ \omega^-}{4} e^{4i\eta} (\beta_+ \alpha_- - \alpha_+ \beta_-) z^4 \prod_{j=1}^N (\bar{n}_j - e^{2i\eta} n_j) (n_j + e^{2i\eta} \bar{n}_j) + \mathcal{O}(z^2), \quad (6.17)$$

$$\Lambda_{\pm}(u) = \pm (-1)^N \frac{\omega^+ \omega^-}{4} e^{4i\eta} (\beta_+ \alpha_- - \alpha_+ \beta_-) z^4 e^{iN 2\eta} + \mathcal{O}(z^2).$$

The eigenvalues $\Lambda_{\pm}(u)$ have been classified according to a parity which is determined by the (diagonal) operator controlling the asymptotics of $\tau(u)$.

Note that in the case of diagonal boundaries, i.e. $\alpha_{\pm} = \beta_{\pm} = 0$, the $\mathcal{O}(z)$ terms of the K matrices become the leading ones such that

$$\begin{aligned} \tau(u) &= -(-1)^N \frac{\omega^+ \omega^-}{4} e^{2i\eta} z^2 \left[e^{i(\psi_+ + \psi_-)} \prod_{j=1}^N (n_j + e^{2i\eta} \bar{n}_j)(n_j + e^{2i\eta} \bar{n}_j) \right. \\ &\quad \left. + e^{-i(\psi_+ + \psi_-)} \prod_{j=1}^N (\bar{n}_j - e^{2i\eta} n_j)(\bar{n}_j - e^{2i\eta} n_j) \right] + \mathcal{O}(z), \\ \Lambda_M(u) &= -(-1)^N \frac{\omega^+ \omega^-}{4} e^{2i\eta} z^2 (e^{i(\psi_+ + \psi_-)} e^{4i(N-M)\eta} + e^{-i(\psi_+ + \psi_-)} e^{4iM\eta}) + \mathcal{O}(z). \end{aligned} \quad (6.18)$$

Here, as in the case of PBC, the asymptotic behavior of the transfer matrix eigenvalues can be related to the (conserved) total number M of particles in the state.

6.3. Fusion of the boundary matrices

For the sake of readability, it is convenient to define the following ordered product of R -matrices,

$$R_i^{\text{string}}(u) \equiv \prod_{k=1}^i R_{k,i+1}(2u + [i+k-1] \cdot 2\eta), \quad (6.19)$$

such that the fused K^- boundary matrices may be written as

$$\begin{aligned} K_{(12\dots n)}^-(u) &\equiv P_{12\dots n}^+ \left[\prod_{i=1}^{n-1} K_i^-(u + [i-1] \cdot 2\eta) R_i^{\text{string}}(u) \right] K_n^-(u + [n-1] \cdot 2\eta) P_{12\dots n}^+ \\ &\Rightarrow A_{(12\dots n)} K_{(12\dots n)}^-(u) A_{(12\dots n)}^{-1} \equiv \left(\begin{array}{c|ccc} K_{\ll 1\dots n \gg}^-(u) & & & \\ \hline & 0 & & \\ & & \ddots & \end{array} \right) \end{aligned} \quad (6.20)$$

(see also [17, 30, 31] for the XXZ model) where $K_{(12\dots n)}^-(u)$ is a $2^n \times 2^n$ -matrix with $K_{\ll 1\dots n \gg}^-(u)$ being the only non-vanishing block of dimensions $(n+1) \times (n+1)$. There is a useful relation between the fused K^- - and K^+ -matrices that stems from (6.7),

$$\begin{aligned} K_{(12\dots n)}^+(u) &= \left[\left(\frac{1}{2 \cos(2\eta)} \right)^n K_{(n\dots 21)}^-(-u - n \cdot 2\eta) \sigma_{(n)}^z \right]_{(\ominus \rightarrow \oplus)} \\ &\Rightarrow A_{(12\dots n)} K_{(12\dots n)}^+(u) A_{(12\dots n)}^{-1} \equiv \left(\begin{array}{c|ccc} K_{\ll 1\dots n \gg}^+(u) & & & \\ \hline & 0 & & \\ & & \ddots & \end{array} \right), \end{aligned} \quad (6.21)$$

and defines the $(n+1) \times (n+1)$ -matrix $K_{\ll 1\dots n \gg}^+(u)$ in the obvious way, where $\sigma_{(n)}^z$ was defined in (3.16). Note that the order of all spaces in $K_{(n\dots 21)}^-$ is inverted. Thus, by changing the space

labels according to $i \rightarrow n + 1 - i$ the fused right boundary matrix may explicitly be written as

$$K_{(12\dots n)}^+(u) = P_{12\dots n}^+ \left[\prod_{i=1}^{n-1} K_{n+1-i}^+(u + [n - i] \cdot 2\eta) \bar{R}_i^{\text{string}}(u) \right] K_1^+(u) P_{12\dots n}^+, \quad (6.22)$$

$$\bar{R}_i^{\text{string}}(u) \equiv \prod_{k=1}^i \bar{R}_{n+1-k, n+1-(i+1)}(-2u + [i + k - 1 - 2n] \cdot 2\eta). \quad (6.23)$$

The reason why the conjugated R -matrices (B.9) appear in this expression is that by commuting the σ^z -matrices, arising from (6.7), to the right, the relation

$$\bar{R}_{ab}(u) = \sigma_a^z R_{ab}(u) \sigma_a^z = \sigma_b^z R_{ab}(u) \sigma_b^z \quad (6.24)$$

is employed, see (B.7).

Since $[P_{(1\dots n)}^+, \sigma_{(n)}^z] = 0$ and $[\sigma_{(n)}^z, A_{(12\dots n)} \sigma_{(n)}^z A_{(12\dots n)}^{-1}] = 0$, the periodicity property (6.5) carries over to the fused K^- -matrices

$$K_{(12\dots n)}^\mp(u + \pi) = (-1)^n \sigma_{(n)}^z K_{(12\dots n)}^\mp(u) \sigma_{(n)}^z, \quad (6.25a)$$

$$K_{\ll 12\dots n \gg}^\mp(u + \pi) = (-1)^n \sigma_{\ll n \gg}^z K_{\ll 12\dots n \gg}^\mp(u) \sigma_{\ll n \gg}^z, \quad (6.25b)$$

where the alternating sign results from successive application of (2.5f).

6.4. Fusion hierarchy for OBC

From the fused quantities, it is again possible to derive a family of commuting operators

$$\tau^{(n)}(u) \equiv \text{str}_{\ll 1\dots n \gg} \left\{ K_{\ll 1\dots n \gg}^+(u) T_{\ll 1\dots n \gg}(u) K_{\ll 1\dots n \gg}^-(u) \hat{T}_{\ll 1\dots n \gg}(u + [n - 1] \cdot 2\eta) \right\} \quad (6.26)$$

that extends the existing family of commuting super transfer matrices $\tau(u) = \tau^{(1)}(u)$ such that $[\tau^{(i)}(u), \tau^{(k)}(v)] = 0$ for all $i, j \geq 1$. The quantity $\hat{T}_{\ll 1\dots n \gg}(u)$ appearing in (6.26) is related to the fused object

$$\begin{aligned} \hat{T}_{(1\dots n)}(u + [n - 1] \cdot 2\eta) &= P_{1\dots n}^+ \hat{T}_1(u) \hat{T}_2(u + 2\eta) \cdot \dots \cdot \hat{T}_n(u + [n - 1] \cdot 2\eta) P_{1\dots n}^+ \\ &= \prod_{i=1}^N \frac{R_{(1\dots n)q_i}(u, \eta)}{\zeta(u) \zeta(u + 2\eta) \cdot \dots \cdot \zeta(u + [n - 1] \cdot 2\eta)} \end{aligned} \quad (6.27)$$

In the usual way by restriction to the only relevant matrix block after applying the respective A -transformation. In the case of general open boundaries, the fusion hierarchy for $n \geq 1$ is found to be

$$\tau^{(n)}(u) \cdot \tau^{(1)}(u + n \cdot 2\eta) = -\frac{\tau^{(n+1)}(u)}{\xi_n(u)} + \frac{\Delta(u + [n - 1] \cdot 2\eta)}{\zeta(2u + 2n \cdot 2\eta)} \cdot \xi_{n-1}(u) \tau^{(n-1)}(u), \quad (6.28)$$

where $\Delta(u)$ labels the OBC SQD defined in (D.23) and

$$\xi_n(u) \equiv \prod_{k=1}^n \zeta(2u + [n + k] \cdot 2\eta). \quad (6.29)$$

The structure of this fusion hierarchy can be further simplified by introducing the rescaled quantities

$$\tilde{\Delta}(u) \equiv \frac{\Delta(u)}{\zeta(2u + 2 \cdot 2\eta)} \quad \text{and} \quad \tilde{\tau}^{(n)}(u) \equiv - \left(\prod_{i=1}^{n-1} \xi_i^{-1}(u) \right) \tau^{(n)}(u) \quad (6.30)$$

with the convenient definitions $\tilde{\tau}^{(0)}(u) \equiv -\tau^{(0)}(u) \equiv \mathbb{1}$ and $\tilde{\tau}^{(1)}(u) \equiv -\tau^{(1)}(u)$ such that (6.28) becomes

$$\tilde{\tau}^{(n)}(u) \cdot \tilde{\tau}^{(1)}(u + n \cdot 2\eta) = \tilde{\tau}^{(n+1)}(u) - \tilde{\Delta}(u + [n - 1] \cdot 2\eta) \cdot \tilde{\tau}^{(n-1)}(u). \quad (6.31)$$

7. TQ-equations for OBC

As in the PBC case, the fusion hierarchy (6.31) provides a system of relations between the eigenvalues $\tilde{\Lambda}^{(n)}(u)$ of the fused (super) transfer matrices. Defining $\tilde{\Lambda}(u) \equiv \tilde{\Lambda}^{(1)}(u)$ and after shifting $u \rightarrow u - n \cdot 2\eta$, this yields

$$\tilde{\Lambda}(u) = \frac{\tilde{\Lambda}^{(n+1)}(u - n \cdot 2\eta)}{\tilde{\Lambda}^{(n)}(u - n \cdot 2\eta)} - \tilde{\Delta}(u - 2\eta) \frac{\tilde{\Lambda}^{(n-1)}(u - n \cdot 2\eta)}{\tilde{\Lambda}^{(n)}(u - n \cdot 2\eta)}. \quad (7.1)$$

Introducing the functions

$$h^{(n)}(u) \gamma^{(n)}(u) \tilde{Q}^{(n)}(u) \equiv \tilde{\Lambda}^{(n)}(u - n \cdot 2\eta), \quad (7.2)$$

where

$$\gamma^{(n)}(u) \equiv \frac{\sin(2u + 2\eta)}{\sin(2u)} \prod_{j=1}^n \frac{\sin(2u - [2j - 2] \cdot 2\eta)}{\sin(2u - [2j - 3] \cdot 2\eta)}, \quad (7.3a)$$

$$h^{(n)}(u) \equiv -(-1)^n \prod_{k=0}^n \omega^+ \sin(u - k \cdot 2\eta - \psi_+) \cdot \omega^- \sin(u - k \cdot 2\eta - \psi_-), \quad (7.3b)$$

the eigenvalues can be written as

$$\begin{aligned} \tilde{\Lambda}(u) &= \mathfrak{K}_\delta^+(u) \mathfrak{K}_\delta^-(u + 2\eta) \frac{\sin(2u)}{\sin(2u + 2\eta)} \frac{\tilde{Q}^{(n+1)}(u + 2\eta)}{\tilde{Q}^{(n)}(u)} \\ &\quad - \frac{\tilde{\Delta}(u - 2\eta)}{\mathfrak{K}_\delta^+(u - 2\eta) \mathfrak{K}_\delta^-(u)} \frac{\sin(2u - 2\eta)}{\sin(2u - 4\eta)} \frac{\tilde{Q}^{(n-1)}(u - 2\eta)}{\tilde{Q}^{(n)}(u)}, \end{aligned} \quad (7.4)$$

where the functions $\mathfrak{K}_{\alpha,\delta}^\pm(u)$ are defined in (C.7). Now assume that the limit $\tilde{Q}(u) \equiv \lim_{n \rightarrow \infty} \tilde{Q}^{(n)}(u)$ exists and can be written as

$$\tilde{Q}(u) = f^N(u) \tilde{q}(u) \quad \text{with} \quad f(u) \equiv e^{i\pi \frac{u}{2\eta}} \frac{\sin(u - 2\eta)}{\sin(u)}. \quad (7.5)$$

Resubstituting $\Lambda(u) = -\tilde{\Lambda}(u)$ by virtue of (6.30), we obtain a TQ-equation for the open small polaron model

$$\Lambda(u) = H_\alpha(u) \frac{\tilde{q}(u - 2\eta)}{\tilde{q}(u)} - H_\delta(u) \frac{\tilde{q}(u + 2\eta)}{\tilde{q}(u)}, \quad (7.6)$$

where the functions $H_\alpha(u)$ and $H_\delta(u)$ factorize the SQD (D.23) as

$$H_\alpha(u) H_\delta(u - 2\eta) = \zeta^{-1}(2u) \Delta(u - 2\eta). \quad (7.7)$$

As discussed in appendix D, the contribution of the boundary matrices to the SQD $\Delta(u)$ of the small polaron model is identical for the diagonal and non-diagonal boundary fields. Therefore, $\Delta(u)$ can be factorized in the parametrization (6.3) giving

$$\begin{aligned} H_\alpha(u) &\equiv \frac{\sin(2u+4\eta)}{\sin(2u+2\eta)} \mathfrak{K}_\alpha^+(u-2\eta) \mathfrak{K}_\alpha^-(u) \left(\frac{-\sin^2(u+2\eta)}{\sin(u+2\eta)\sin(u-2\eta)} \right)^N, \\ H_\delta(u) &\equiv \frac{\sin(2u)}{\sin(2u+2\eta)} \mathfrak{K}_\delta^+(u) \mathfrak{K}_\delta^-(u+2\eta) \left(\frac{-\sin^2(u)}{\sin(u+2\eta)\sin(u-2\eta)} \right)^N. \end{aligned} \quad (7.8)$$

With this factorization of the SQD the TQ-equation (7.6) coincides with the known result (C.9) for the diagonal boundary case obtained by means of the algebraic or coordinate Bethe ansatz [13–15]. In this case the spectral problem for the M -particle sector of the small polaron model can be solved using the factorized ansatz (C.8)

$$\tilde{q}(u) = \prod_{\ell=1}^M \sin(u+2\eta+\nu_\ell) \sin(u-\nu_\ell), \quad (7.9)$$

where the unknown parameters ν_ℓ , $\ell = 1, \dots, M$, have to satisfy the Bethe equations (C.5).

For generic non-diagonal boundary matrices, an ansatz (7.9) leads to a constraint on the boundary parameters (and the number M) which guarantees consistency between the asymptotic behavior of the right-hand side of (7.6) and the known behavior of the transfer matrix eigenvalues $\Lambda_\pm(u)$ (6.17). Using such a requirement, Bethe equations have been formulated for the spectral problem of open (non-diagonal) XXZ and XYZ Heisenberg spin chains [20, 27, 28]. Unfortunately, in the present case of the small polaron model, the factorization (7.8) of the quantum determinant does not reproduce the leading asymptotic behavior of the transfer matrix eigenvalues for any non-diagonal boundary fields.

To proceed with the solution of the TQ-equation (7.6), one has to find a different factorization of the quantum determinant satisfying (7.7) or to modify the ansatz (7.9) for the Q -functions. Based on the dependence of the transfer matrix on the off-diagonal boundary parameters in various limits (6.15), (6.17) and observations for small system sizes, we propose that the Q -functions can be written as

$$\tilde{q}(u) = q(u) + \rho(u) (\beta_+ \alpha_- - \alpha_+ \beta_-) \quad (7.10)$$

in the case of non-diagonal boundary conditions with $q(u)$ being the factorized expression (7.9) as in the diagonal case and another unknown function $\rho(u)$ depending on the anisotropy η and the diagonal boundary parameters ψ_\pm . To determine $\rho(u)$ the ansatz (7.10) should be used in the TQ-equation (7.6) together with the analytical properties of the transfer matrix eigenvalues, in particular their asymptotic behavior (6.17).

8. Truncation of the OBC fusion hierarchy

From here on, for the sake of readability, some of the functions introduced above will be equipped with a second parameter indicating for them to be taken at that particular value of the anisotropy η . For instance, $K^\pm(u, \rho) \equiv K^\pm(u)|_{\eta \rightarrow \rho}$ and so on and so forth.

8.1. K -matrix truncation

It is convenient to define the following functions,

$$\mu_n^\pm(u) \equiv \pm \delta \{K^\pm(\mp u - 2\eta_n, \eta_n)\} \frac{\sin(2\eta_n)}{\sin(2u - 2 \cdot 2\eta_n)} \prod_{k=2}^{2n} \frac{\sin(2u + k \cdot 2\eta_n)}{\sin(2\eta_n)}, \quad (8.1)$$

$$v_n^\pm(u) \equiv \mp \frac{\omega_n^\pm}{\mu_n^\pm(u)} \left(\frac{\omega_n^\pm}{2}\right)^n \sin([n+1][u \mp \psi_\pm]) \prod_{i=1}^n \prod_{j=1}^i \frac{\sin(2u + [i+j] \cdot 2\eta_n)}{\sin(2\eta_n)}, \quad (8.2)$$

where $\omega_n^\pm \equiv \omega^\pm(\eta_n)$ and to introduce the shorthand notations

$$\begin{aligned} \mathcal{K}_{\ll n \gg}^-(u, \eta) &\equiv \sigma_{\ll n \gg}^z \cdot K_{\ll 1 \dots n \gg}^-(u + 2\eta), \\ \mathcal{K}_{\ll n \gg}^+(u, \eta) &\equiv K_{\ll 1 \dots n \gg}^+(u + 2\eta) \cdot \sigma_{\ll n \gg}^z. \end{aligned} \quad (8.3)$$

The truncation identities for the boundary matrices can then be expressed as

$$\begin{aligned} C_{\ll 1 \dots n \gg} K_{\ll 1 \dots n \gg}^\pm(u, \eta_{n-1}) C_{\ll 1 \dots n \gg}^{-1} \\ = \mu_{n-1}^\pm(u) \left(\begin{array}{c} v_{n-1}^\pm(\mp u) \\ B_{\ll 1 \dots n-2 \gg} \mathcal{K}_{\ll n-2 \gg}^\pm(u, \eta_{n-1}) B_{\ll 1 \dots n-2 \gg}^{-1} \\ (\pm 1)^n v_{n-1}^\pm(\pm u) \end{array} \right). \end{aligned} \quad (8.4)$$

8.2. OBC super transfer matrix truncation

In order to be compatible with the truncation identities for the boundary matrices, the R -matrix truncation identities (5.2) need to be recast, this time employing the C transformation matrices

$$\begin{aligned} C_{\ll 1 \dots n \gg} R_{\ll 1 \dots n \gg q}(u, \eta_{n-1}) C_{\ll 1 \dots n \gg}^{-1} \\ = \left(\begin{array}{c} -\mathcal{M}_{n-1}(u) \sigma_q^z \\ \zeta(u) \sigma_q^z \mathcal{R}_q^{(n-2)}(u + 2\eta_{n-1}, \eta_{n-1}) \\ \mathcal{M}_{n-1}(u) (\sigma_q^z)^{n-1} \end{array} \right), \end{aligned} \quad (8.5)$$

where in slight contrast to definition (5.3)

$$\mathcal{R}_q^{(n)}(u, \eta) \equiv B_{\ll 1 \dots n \gg} R_{\ll 1 \dots n \gg q}(u) B_{\ll 1 \dots n \gg}^{-1} \quad (8.6)$$

such that for the single row monodromy matrix

$$\mathcal{T}^{(n)}(u, \eta) \equiv C_{\ll 1 \dots n \gg} R_{\ll 1 \dots n \gg q_N}(u) \cdot \dots \cdot R_{\ll 1 \dots n \gg q_2}(u) R_{\ll 1 \dots n \gg q_1}(u) C_{\ll 1 \dots n \gg}^{-1} \quad (8.7)$$

$$\equiv C_{\ll 1 \dots n \gg} T_{\ll 1 \dots n \gg}(u) C_{\ll 1 \dots n \gg}^{-1}, \quad (8.8)$$

the truncation identity at $\eta = \eta_{n-1}$ reads

$$\begin{aligned} \mathcal{T}^{(n)}(u, \eta_{n-1}) \\ = \left(\begin{array}{c} [-\mathcal{M}_{n-1}(u)]^N \prod_{i=N}^1 \sigma_{q_i}^z \\ \zeta^N(u) \prod_{i=N}^1 \sigma_{q_i}^z \mathcal{R}_{q_i}^{(n-2)}(u + 2\eta_{n-1}, \eta_{n-1}) \\ [\mathcal{M}_{n-1}(u)]^N \prod_{i=N}^1 (\sigma_{q_i}^z)^{n-1} \end{array} \right). \end{aligned} \quad (8.9)$$

Again it is convenient to introduce the C -transformed object

$$\widehat{\mathcal{T}}^{(n)}(u, \eta) \equiv C_{\ll 1 \dots n \gg} \widehat{T}_{\ll 1 \dots n \gg}(u) C_{\ll 1 \dots n \gg}^{-1} \quad (8.10)$$

to easily recognize the truncation identity

$$\begin{aligned} \widehat{\mathcal{T}}^{(n)}(u + [n - 1] \cdot 2\eta_{n-1}, \eta_{n-1}) &= \frac{1}{\zeta^N(u) \zeta^N(u + 2\eta_{n-1}) \dots \zeta^N(u + [n - 1] \cdot 2\eta_{n-1})} \\ &\times \left(\begin{array}{c} [-\mathcal{M}_{n-1}(u)]^N \prod_{i=1}^N \sigma_{q_i}^z \\ \zeta^N(u) \prod_{i=1}^N \sigma_{q_i}^z \mathcal{R}_{q_i}^{(n-2)}(u + 2\eta_{n-1}, \eta_{n-1}) \\ [\mathcal{M}_{n-1}(u)]^N \prod_{i=1}^N (\sigma_{q_i}^z)^{n-1} \end{array} \right). \end{aligned} \quad (8.11)$$

Now that the individual truncation identities for all the objects involved in the construction of the fused OBC super transfer matrix $\tau^{(n)}(u)$ are known, it can be shown by simple matrix multiplication⁶ of (8.4⁺), (8.9), (8.4⁻) and (8.11) that

$$\tau^{(n)}(u, \eta_{n-1}) = \text{str}_{\ll 1 \dots n \gg} \left\{ \begin{pmatrix} X^+ & & \\ & Y & * \\ & & X^- \end{pmatrix} \right\} = X^+ - \text{str}_{\ll 1 \dots n-2 \gg} \{ Y \} + (-1)^n X^- \quad (8.12)$$

with the placeholders X^\pm and Y defined by

$$X^\pm \equiv (\pm 1)^n \left[\prod_{k=0}^{n-1} \zeta^{-N}(u + k \cdot 2\eta_{n-1}) \right] \mathcal{M}_{n-1}^{2N}(u) \mu_{n-1}^+(u) \mu_{n-1}^-(u) v_{n-1}^+(\mp u) v_{n-1}^-(\pm u) \quad (8.13)$$

and

$$\begin{aligned} Y &= \phi_{n-1}^\tau(u) B_{\ll 1 \dots n-2 \gg} K_{\ll 1 \dots n-2 \gg}^+(u + 2\eta_{n-1}) \sigma_{\ll n-2 \gg}^z \left(\prod_{i=1}^N \sigma_{q_i}^z \right) \\ &\times T_{\ll 1 \dots n-2 \gg}(u + 2\eta_{n-1}) \sigma_{\ll n-2 \gg}^z K_{\ll 1 \dots n-2 \gg}^-(u + 2\eta_{n-1}) \\ &\times \left(\prod_{i=1}^N \sigma_{q_i}^z \right) \widehat{T}_{\ll 1 \dots n-2 \gg}(u + 2\eta_{n-1} + [(n-2) - 1] \cdot 2\eta_{n-1}) B_{\ll 1 \dots n-2 \gg}^{-1} \\ &= \phi_{n-1}^\tau(u) B_{\ll 1 \dots n-2 \gg} K_{\ll 1 \dots n-2 \gg}^+(u + 2\eta_{n-1}) T_{\ll 1 \dots n-2 \gg}(u + 2\eta_{n-1}) \\ &\times K_{\ll 1 \dots n-2 \gg}^-(u + 2\eta_{n-1}) \widehat{T}_{\ll 1 \dots n-2 \gg}(u + 2\eta_{n-1} + [(n-2) - 1] \cdot 2\eta_{n-1}) B_{\ll 1 \dots n-2 \gg}^{-1}. \end{aligned} \quad (8.14)$$

In the second step of equation (8.14), relation (D.22) has been employed to get rid of the σ^z factors such that (8.12) eventually yields the truncation identities for the OBC transfer matrices,

$$\tau^{(n)}(u, \eta_{n-1}) = \phi_{n-1}^{\text{id}}(u) \cdot \mathbb{1} - \phi_{n-1}^\tau(u) \cdot \tau^{(n-2)}(u + 2\eta_{n-1}, \eta_{n-1}), \quad (8.15)$$

where $\phi_n^{\text{id}}(u)$ and $\phi_n^\tau(u)$ are rather lengthy expressions given by

$$\begin{aligned} \phi_n^{\text{id}}(u) &= \left[\prod_{k=0}^n \zeta^{-N}(u + k \cdot 2\eta_n) \right] \mathcal{M}_n^{2N}(u) \mu_n^+(u) \mu_n^-(u) [v_n^+(-u) v_n^-(u) + v_n^+(u) v_n^-(-u)], \\ \phi_n^\tau(u) &= \left(\frac{\zeta(u)}{\zeta(u + n \cdot 2\eta_n)} \right)^N \mu_n^+(u) \mu_n^-(u). \end{aligned} \quad (8.16)$$

⁶ Due to the cyclic invariance of the supertrace, all the matrix objects in (6.26) may be conjugated by means of the C -transformation without changing the actual super transfer matrix.

In terms of the rescaled transfer matrices (6.31) it is reasonable to introduce

$$\begin{aligned}\tilde{\phi}_n^{\text{id}}(u) &= - \left[\prod_{i=1}^n \xi_i^{-1}(u) \right]_{\eta=\eta_n} \phi_n^{\text{id}}(u), \\ \tilde{\phi}_n^{\tau}(u) &= \left[\prod_{i=1}^n \xi_i^{-1}(u) \right]_{\eta=\eta_n} \phi_n^{\tau}(u) \left[\prod_{i=1}^{n-2} \xi_i(u + 2\eta_n) \right]_{\eta=\eta_n},\end{aligned}\tag{8.17}$$

which yield the respective rescaled truncation identities

$$\tilde{\tau}^{(n)}(u, \eta_{n-1}) = \tilde{\phi}_{n-1}^{\text{id}}(u) \cdot \mathbb{1} - \tilde{\phi}_{n-1}^{\tau}(u) \cdot \tilde{\tau}^{(n-2)}(u + 2\eta_{n-1}, \eta_{n-1}).\tag{8.18}$$

9. Summary and conclusion

Starting from structures provided by the YBA (2.6) and the reflection algebra (6.1), (6.2), we have set up the fusion hierarchies for the commuting transfer matrices $\tau^{(n)}(u)$ of the small polaron model with periodic and general open boundary conditions, respectively. Following previous work on spin chains with non-diagonal boundary fields [20, 27, 28], we have obtained TQ-equations for the eigenvalues of the transfer matrices by assuming the limit $n \rightarrow \infty$ of these expressions to exist. These TQ-equations can be solved by functional Bethe ansatz methods in the case of periodic and diagonal open boundary conditions. The resulting spectrum coincides with what has been found previously using the algebraic Bethe ansatz [4, 5, 13–15] and was to be expected as a consequence of the Jordan–Wigner equivalence of the small polaron model with the spin-1/2 XXZ Heisenberg chain.

For generic non-diagonal boundary conditions, the $U(1)$ symmetry of the model corresponding to particle number conservation is broken. Therefore, the algebraic approach cannot be applied as it uses the Fock vacuum as a reference state and relies on this being an eigenstate of the system. This situation is well known from the (ungraded) spin-1/2 XXZ Heisenberg chain with non-diagonal boundary fields where in spite of significant activities a practical solution of the eigenvalue problem for generic anisotropies and boundary fields is lacking. Here we have used the strategies employed previously for the XXZ chain to the (graded) small polaron chain: apart from the formulation of the spectral problem in terms of a TQ-equation, the fusion hierarchy can be truncated at a finite order for anisotropies being roots of unity, $\eta_p = \pi/(2(p+1))$ [17]. We have derived the corresponding truncation identities for the small polaron model subject to all boundary conditions considered. Inspection of the R -matrices obtained at the first few fusion levels suggests that it is possible to derive similar identities for anisotropies given by integer multiples of η_p .

To actually compute eigenvalues of the transfer matrices, further steps have to be taken: for anisotropies being roots of unity, the truncated fusion hierarchy can be analyzed following the steps that have been established for the XXZ chain [33–35] where additional constraints on the boundary fields may arise. For generic anisotropies the situation is more complicated: in the ungraded XXZ chain, a (factorized) Bethe ansatz for the Q -function given in terms of finitely many parameters such as (7.9) was possible only if the boundary parameters satisfy a constraint [18–20, 23, 28]. For graded models such a constraint may be absent: in the rational limit $\eta \rightarrow 0$ of the model considered here, the functional form of the Q -function remained unchanged when off-diagonal boundary fields were added [26]. Similarly, the nilpotency of the off-diagonal boundary fields may allow for a general solution of the small polaron model.

As shown in appendix D, the SQD of this model depends only on the diagonal boundary parameters which simplifies the factorization problem (7.7). In addition, the odd Grassmann numbers parametrizing the off-diagonal boundary fields appear only in a specific combination. Therefore, starting with the proposed ansatz (7.10) for the Q -function, the derivation of Bethe-type equations appears to be possible in the generic case. These open questions shall be addressed in a future publication.

A possible extension of the present work is to consider integrable higher spin chains with generic boundary conditions. Such generalizations of an integrable model can be constructed by application of the fusion method [29–31] in the quantum spaces of the model in addition to fusion in auxiliary space as used in this paper for the derivation of the fusion hierarchies (3.20) and (6.31). Starting from the spin-1/2 XXZ Heisenberg chain, this leads to the hierarchy of integrable higher spin XXZ models [36–38] including the spin-1 Fateev–Zamolodchikov model [39, 40]. Similarly, this method has been used for the construction and solution of graded models based on higher spin representations of super Lie algebras, see e.g. [41–45]. In the present context this would lead to integrable generalizations of the small polaron model with general boundary conditions. The local Hilbert spaces of these models have dimension $(n/2|n/2)$ for n even and $((n+1)/2|(n-1)/2)$ for n odd, see table 1. A quantum chain with local interactions can be constructed from R -matrices acting on the tensor product of two copies of such a space. The integrable open boundary conditions for these models are given in terms of the fused K -matrices (6.20). Taking into account the gradation, the possible states can be identified e.g. with the internal degrees of freedom of a fermionic lattice model with several local orbitals to allow for a physical interpretation of the resulting quantum chain. For the higher spin XXZ models with general open boundary conditions, the spectral problem has been studied by Frappat *et al* [28] who found that the solution requires similar constraints as in the spin-1/2 case.

Acknowledgments

We thank Nikos Karaiskos for useful discussions on the subject of this paper. This work has been supported by the Deutsche Forschungsgemeinschaft under grant no. Fr 737/6.

Appendix A. Graded vector spaces

Fermionic lattice models exhibit a natural \mathbb{Z}_2 gradation on their local space of states, i.e. $V = V_0 \oplus V_1$ is equipped with a notion of parity,

$$p : V_i \rightarrow \mathbb{Z}_2, \quad p(v_i) \mapsto i \in \{0, 1\}. \quad (\text{A.1})$$

Let $\dim V_0 \equiv m \in \mathbb{N}$ and $\dim V_1 \equiv n \in \mathbb{N}$ be finite. Then V is said to have dimension $(m|n)$ and V_0, V_1 are called the *homogeneous subspaces* of V . An element $v \in V$ is said to be *even* if $p(v) = 0$ and is, respectively, called *odd* if $p(v) = 1$. While even elements of V correspond to bosonic states, odd elements represent fermionic states. For instance, consider the case where both of the homogeneous subspaces V_0 and V_1 are one dimensional such that the composite local space of states $V = V_0 \oplus V_1$ is spanned by just one bosonic and one fermionic state. Then V is said to have *BF*-grading, where *BF* refers to an ordered basis of V in which the first basis vector is associated with the bosonic state (*B*) whereas the second basis vector is associated

with the fermionic state (F). Now consider the tensor product of two copies of V . Taking into account the order of the basis states, the tensor product space will have $BFFB$ -grading,

$$V \otimes V = (V_0 \oplus V_1) \otimes (V_0 \oplus V_1) = \underbrace{(V_0 \otimes V_0)}_B \oplus \underbrace{(V_0 \otimes V_1)}_F \oplus \underbrace{(V_1 \otimes V_0)}_F \oplus \underbrace{(V_1 \otimes V_1)}_B. \quad (\text{A.2})$$

In the following, the conventions from [46] will essentially be adopted.

Let $\{e_1, e_2, \dots, e_m, e_{m+1}, \dots, e_{m+n}\}$ be a homogeneous basis of V , i.e. each basis element has distinct parity $p(e_\alpha)$, and for convenience let this basis be ordered, such that the first m elements span the even and the last n elements span the odd subspace of V ,

$$p(\alpha) \equiv p(e_\alpha) = \begin{cases} 0 & \text{if } 1 \leq \alpha \leq m, \\ 1 & \text{if } m+1 \leq \alpha \leq m+n. \end{cases} \quad (\text{A.3})$$

In order to deal with an algebra of linear operators, acting on the graded local space of states, it is necessary to extend the concept of parity to $\text{End}(V)$, the space of endomorphisms of V . The $(m+n) \times (m+n)$ basis elements of $\text{End}(V)$ will be labeled e_α^β and are defined through their action on the above basis of V ,

$$e_\alpha^\beta e_\gamma \equiv \delta_\gamma^\beta e_\alpha. \quad (\text{A.4})$$

By extending the definition of the parity function to

$$p(e_\alpha^\beta) \equiv p(\alpha) + p(\beta) \pmod{2}, \quad (\text{A.5})$$

$\text{End}(V)$ becomes a \mathbb{Z}_2 graded vector space. A basis of the N -fold product space

$$\text{End}^{\otimes N}(V) \equiv \underbrace{\text{End}(V) \otimes \text{End}(V) \otimes \dots \otimes \text{End}(V)}_{N \text{ times}} \quad (\text{A.6})$$

can most naturally be obtained by embedding the local basis elements e_α^β into this tensor product structure. Moreover, $\text{End}^{\otimes N}(V)$ acquires a \mathbb{Z}_2 grading by a further extension of the definition of the parity function,

$$p(e_{\alpha_1}^{\beta_1} \otimes e_{\alpha_2}^{\beta_2} \otimes \dots \otimes e_{\alpha_N}^{\beta_N}) \equiv p(e_{\alpha_1}^{\beta_1}) + p(e_{\alpha_2}^{\beta_2}) + \dots + p(e_{\alpha_N}^{\beta_N}) \pmod{2}. \quad (\text{A.7})$$

When dealing with graded vector spaces, it is useful to replace the usual tensor product structure by a so-called *super tensor product*. The symbol \otimes_s will be used to distinguish this new structure. With respect to a certain basis, the components of the super tensor product of two operators $A \in \text{End}^{\otimes k}(V)$ and $B \in \text{End}^{\otimes l}(V)$, where $k, l \in \mathbb{N}$, are explicitly defined through

$$(A \otimes_s B)_{\beta\delta}^{\alpha\gamma} = (-1)^{[p(\alpha)+p(\beta)]p(\gamma)} A_\beta^\alpha B_\delta^\gamma. \quad (\text{A.8})$$

As pointed out in [46], the super tensor product allows for a most convenient *graded* embedding of the e_α^β into the j th subspace of $\text{End}^{\otimes N}(V)$,

$$e_{j,\alpha}^\beta \equiv \mathbb{1}^{\otimes(j-1)} \otimes_s e_\alpha^\beta \otimes_s \mathbb{1}^{\otimes(N-j)}. \quad (\text{A.9})$$

A graded version of the permutation operator \mathcal{P} is defined by the relation

$$\mathcal{P}(A \otimes_s B) = (B \otimes_s A)\mathcal{P}. \quad (\text{A.10})$$

If (A.9) is employed as a basis for $\text{End}^{\otimes N}(V)$, the operator \mathcal{P}_{ij} which permutes the i th and the j th subspace can explicitly be constructed as

$$\mathcal{P}_{ij} = (-1)^{p(\beta)} e_{i,\alpha}^\beta e_{j,\beta}^\alpha. \quad (\text{A.11})$$

In the following, the definitions of some well-known operations, namely the matrix transposition and the trace operation, will be adapted to fit the needs of graded vector spaces. A nicely motivated and much more elaborate list of matrix operations on graded vector spaces can be found in [16].

- Firstly, the *super transposition* of an element $A \in \text{End}(V)$ is defined by

$$(A^{\text{st}})_{\beta}^{\alpha} = (-1)^{p(\alpha)[p(\alpha+\beta)]} A_{\beta}^{\alpha}. \quad (\text{A.12})$$

In contrast to the ungraded case, the super transposition is not an involution, i.e. applying the super transposition twice does not yield the identity operation. As pointed out in [8], it is therefore convenient to introduce an *inverse super transposition*,

$$(A^{\text{ist}})_{\beta}^{\alpha} = (-1)^{p(\beta)[p(\alpha+\beta)]} A_{\beta}^{\alpha}. \quad (\text{A.13})$$

The *partial super transposition*, i.e. a super transposition on the j th subspace of $\text{End}^{\otimes N}(V)$, is defined through

$$(A_1 \otimes_s \cdots \otimes_s A_j \otimes_s \cdots \otimes_s A_N)^{\text{st}j} \equiv A_1 \otimes_s \cdots \otimes_s (A_j)^{\text{st}} \otimes_s \cdots \otimes_s A_N. \quad (\text{A.14})$$

The partial inverse super transposition is defined analogously. Note that, as opposed to ordinary partial matrix transpositions on ungraded vector spaces, the successive application of partial super transpositions on all subspaces is generally not equal to a total super transposition, i.e. $(A_1 \otimes_s A_2)^{\text{st}_1 \text{st}_2} \neq (A_1 \otimes_s A_2)^{\text{st}}$.

- Secondly, the *super trace* of some $A \in \text{End}(V)$ is given by

$$\text{str} \{ A \} \equiv \sum_{\alpha} (-1)^{p(\alpha)} A_{\alpha}^{\alpha}. \quad (\text{A.15})$$

For operators $B \in \text{End}^{\otimes N}(V)$, it is convenient to define a *partial super trace* on subspace j as

$$\text{str}_j \{ B \}_{\beta_1 \dots \beta_{j-1} \beta_{j+1} \dots \beta_N}^{\alpha_1 \dots \alpha_{j-1} \alpha_{j+1} \dots \alpha_N} \equiv \sum_{\gamma} (-1)^{p(\gamma)} B_{\beta_1 \dots \beta_{j-1} \gamma \beta_{j+1} \dots \beta_N}^{\alpha_1 \dots \alpha_{j-1} \gamma \alpha_{j+1} \dots \alpha_N}. \quad (\text{A.16})$$

Appendix B. Relation to Bracken's dual reflection algebra

According to [8] the dual reflection equation for quite general graded models reads

$$\begin{aligned} R_{12}(v-u) K_1^+(u) \tilde{\tilde{R}}_{21}(-u-v)^{\text{ist}_1 \text{st}_2} K_2^+(v) \\ = K_2^+(v) \tilde{\tilde{R}}_{12}(-u-v)^{\text{ist}_1 \text{st}_2} K_1^+(u) R_{21}(v-u), \end{aligned} \quad (\text{B.1})$$

where

$$\tilde{\tilde{R}}_{21}(\lambda)^{\text{ist}_1 \text{st}_2} = \left(\left[\{ R_{21}^{-1}(\lambda) \}^{\text{ist}_2} \right]^{-1} \right)^{\text{st}_2}, \quad (\text{B.2})$$

$$\tilde{\tilde{R}}_{12}(\lambda)^{\text{ist}_1 \text{st}_2} = \left(\left[\{ R_{12}^{-1}(\lambda) \}^{\text{st}_1} \right]^{-1} \right)^{\text{ist}_1}. \quad (\text{B.3})$$

By performing a super transposition on the first space and an inverse super transposition on the second, i.e. by applying $(\cdot)^{st_1 ist_2}$ to equation (B.1), one obtains the equivalent form

$$\begin{aligned} & R_{21}(v-u)^{st_1 ist_2} K_1^+(u)^{st_1} \tilde{R}_{12}(-u-v) K_2^+(v)^{ist_2} \\ &= K_2^+(v)^{ist_2} \tilde{R}_{21}(-u-v) K_1^+(u)^{st_1} R_{12}(v-u)^{st_1 ist_2}. \end{aligned} \tag{B.4}$$

In the case of the small polaron R -matrix as defined in (2.3), one finds

$$\tilde{R}_{21}(\lambda) = \frac{\zeta(\lambda)}{\zeta(\lambda - 2\eta)} R_{12}(\lambda - 4\eta), \tag{B.5}$$

$$\tilde{R}_{12}(\lambda) = \frac{\zeta(\lambda)}{\zeta(\lambda - 2\eta)} R_{21}(\lambda - 4\eta). \tag{B.6}$$

At this point it is convenient to introduce a shorthand, which will henceforth be referred to as a *conjugated R -matrix*,

$$\bar{R}_{ba}(\lambda) \equiv M_a^{-1} R_{ba}(\lambda) M_a \tag{B.7}$$

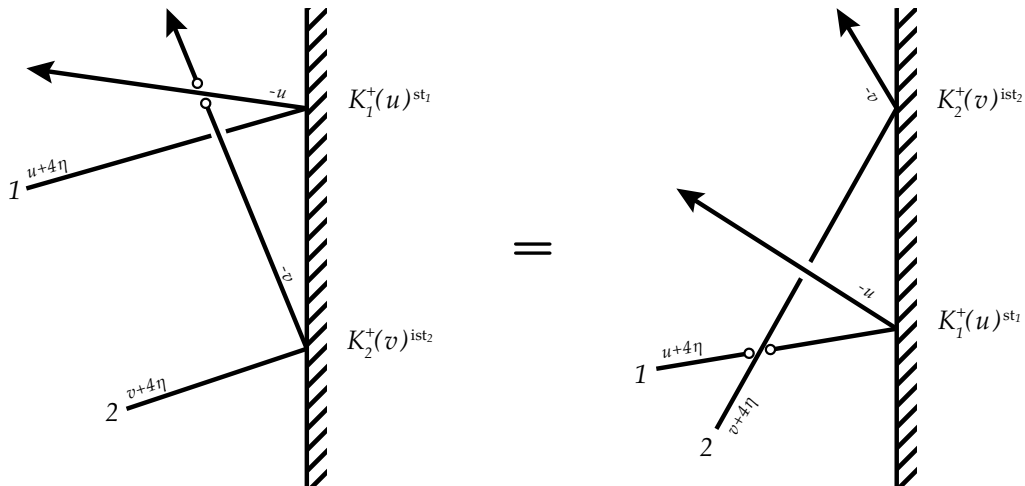
with M being the so-called crossing matrix. For the small polaron model in particular, it is found that $M = \sigma^z$ such that

$$\begin{aligned} \bar{R}_{ab}(\lambda) &= R_{ba}^{st_a ist_b}(\lambda) \stackrel{(2.5a)}{=} R_{ba}^{ist_a st_b}(\lambda) \\ &= R_{ab}^{st_a^2}(\lambda) = R_{ab}^{ist_a^2}(\lambda) = R_{ab}^{st_b^2}(\lambda) = R_{ab}^{ist_b^2}(\lambda). \end{aligned} \tag{B.8}$$

Using this conjugated R -matrix (B.8), the dual reflection equation may be written as

$$\begin{aligned} & \bar{R}_{12}(v-u) K_1^+(u)^{st_1} R_{21}(-u-v-4\eta) K_2^+(v)^{ist_2} \\ &= K_2^+(v)^{ist_2} R_{12}(-u-v-4\eta) K_1^+(u)^{st_1} \bar{R}_{21}(v-u) \end{aligned} \tag{B.9}$$

and is graphically depicted by



Appendix C. Algebraic Bethe ansatz for diagonal boundaries

The reflection equation (6.1) gives 16 fundamental commutation relations for the quantum space operators \mathcal{A} , \mathcal{B} , \mathcal{C} and \mathcal{D} , of which the following three are of particular interest,

$$\mathcal{B}(u)\mathcal{B}(v) = \mathcal{B}(v)\mathcal{B}(u), \quad (\text{C.1})$$

$$\begin{aligned} \mathcal{A}(u)\mathcal{B}(v) &= \frac{s_0(u+v)s_2(v-u)}{s_0(v-u)s_2(u+v)}\mathcal{B}(v)\mathcal{A}(u) \\ &+ \frac{\vartheta(v)s_2(0)}{s_2(u+v)}\mathcal{B}(u) \left\{ \frac{s_0(2v)s_2(u+v)}{\vartheta(v)s_0(u-v)s_2(2v)}\mathcal{A}(v) - \tilde{\mathcal{D}}(v) \right\}, \end{aligned} \quad (\text{C.2})$$

$$\begin{aligned} \tilde{\mathcal{D}}(u)\mathcal{B}(v) &= \frac{s_4(u+v)s_2(u-v)}{s_0(u-v)s_2(u+v)}\mathcal{B}(v)\tilde{\mathcal{D}}(u) - \frac{s_2(0)s_4(2u)s_0(2v)}{\vartheta(u)s_2(2u)s_2(u+v)s_2(2v)}\mathcal{B}(u) \\ &\times \left\{ \frac{\vartheta(v)s_2(2v)s_2(u+v)}{s_0(2v)s_0(u-v)}\tilde{\mathcal{D}}(v) - \mathcal{A}(v) \right\}, \end{aligned} \quad (\text{C.3})$$

using the abbreviation $s_k(\lambda) \equiv \sin(\lambda + k\eta)$. To obtain the desired commutation relations, it is necessary to make an ansatz for a shifted \mathcal{D} -operator

$$\mathcal{D}(\lambda) = \vartheta(\lambda)\tilde{\mathcal{D}}(\lambda) + \phi(\lambda)\mathcal{A}(\lambda) \quad (\text{C.4})$$

and to determine the scalar functions $\phi(\lambda)$ and $\vartheta(\lambda)$. It turns out that $\phi(\lambda) = \frac{s_2(0)}{s_2(2\lambda)}$ while $\vartheta(\lambda)$ remains arbitrary. Starting from the general boundary matrices given in (6.3), the diagonal case can easily be obtained by setting $\alpha_{\pm} = \beta_{\pm} = 0$. This leads to Bethe equations

$$\left(\frac{s_2(v_j)}{s_0(v_j)} \right)^{2N} = \frac{s_2(v_j - \psi_+)s_2(v_j - \psi_-)}{s_0(v_j + \psi_+)s_0(v_j + \psi_-)} \prod_{\substack{\ell=1 \\ \ell \neq j}}^M \frac{s_4(v_j + v_\ell)s_2(v_j - v_\ell)}{s_0(v_j + v_\ell)s_{-2}(v_j - v_\ell)} \quad (\text{C.5})$$

and super transfer matrix eigenvalues⁷

$$\begin{aligned} \Lambda(u) &= \mathfrak{K}_{\alpha}^{-}(u) \left(\mathfrak{K}_{\alpha}^{+}(u) - \frac{s_2(0)}{s_2(2u)}\mathfrak{K}_{\delta}^{+}(u) \right) \left(\frac{s_2(u)}{s_2(-u)} \right)^N \prod_{\ell=1}^M \frac{s_0(u+v_\ell)s_2(v_\ell-u)}{s_0(v_\ell-u)s_2(u+v_\ell)} \\ &- \mathfrak{K}_{\delta}^{+}(u) \left(\mathfrak{K}_{\delta}^{-}(u) - \frac{s_2(0)}{s_2(2u)}\mathfrak{K}_{\alpha}^{-}(u) \right) \left(\frac{s_0^2(u)}{s_2(u)s_2(-u)} \right)^N \prod_{\ell=1}^M \frac{s_4(u+v_\ell)s_2(u-v_\ell)}{s_0(u-v_\ell)s_2(u+v_\ell)}. \end{aligned} \quad (\text{C.6})$$

Here $\mathfrak{K}_{\alpha,\delta}^{\pm}(u)$ label the diagonal entries of the boundary matrices (6.3),

$$\begin{aligned} \mathfrak{K}_{\alpha}^{-}(u) &= \omega^{-} \sin(\psi_- + u), & \mathfrak{K}_{\alpha}^{+}(u) &= \omega^{+} \sin(u + 2\eta + \psi_+), \\ \mathfrak{K}_{\delta}^{-}(u) &= \omega^{-} \sin(\psi_- - u), & \mathfrak{K}_{\delta}^{+}(u) &= \omega^{+} \sin(u + 2\eta - \psi_+). \end{aligned} \quad (\text{C.7})$$

⁷ Note that this result corresponds to the one obtained by Umeno *et al* [13]. However, the authors of [13] seem to have made a slight mistake when substituting their formula (57) into (61) to obtain (62), which should correctly read

$$t(u) = + \frac{\sin(2u+4\eta) \sin(u+t^+)}{\sin(2u+2\eta)} \mathcal{A}(u) - \frac{\sin(u+2\eta-t^+)}{\sin(2u+2\eta)} \tilde{\mathcal{D}}(u).$$

Introducing the functions

$$q(u) \equiv \prod_{\ell=1}^M \sin(u + 2\eta + v_\ell) \sin(u - v_\ell), \quad (\text{C.8})$$

the eigenvalues (C.6) can be recast as

$$\begin{aligned} \Lambda(u)q(u) &= \mathfrak{K}_\alpha^-(u) \left(\mathfrak{K}_\alpha^+(u) - \frac{s_2(0)}{s_2(2u)} \mathfrak{K}_\delta^+(u) \right) \left(\frac{s_2^2(u)}{s_2(u)s_2(-u)} \right)^N q(u - 2\eta) \\ &\quad - \mathfrak{K}_\delta^+(u) \left(\mathfrak{K}_\delta^-(u) - \frac{s_2(0)}{s_2(2u)} \mathfrak{K}_\alpha^-(u) \right) \left(\frac{s_2^2(u)}{s_2(u)s_2(-u)} \right)^N q(u + 2\eta). \end{aligned} \quad (\text{C.9})$$

Appendix D. Super quantum determinants

Consider a generic $BFFB$ graded R -matrix of the shape

$$R(u) = \begin{pmatrix} a(u+2\eta) & 0 & 0 & 0 \\ 0 & a(u) & a(2\eta) & 0 \\ 0 & a(2\eta) & a(u) & 0 \\ 0 & 0 & 0 & -a(u+2\eta) \end{pmatrix}, \quad (\text{D.1})$$

where $a(-u) = a(u)$ and $a(0) = 0$. At $u = -2\eta$ such an R -matrix gives rise to a projector P^- onto a one-dimensional subspace

$$P^- = -\frac{1}{2a(2\eta)} R(-2\eta) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1/2 & -1/2 & 0 \\ 0 & -1/2 & 1/2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (\text{D.2})$$

Let $T(u)$ be a representation of the graded YBA

$$R_{12}(u-v) T_1(u) T_2(v) = T_2(v) T_1(u) R_{12}(u-v) \quad (\text{D.3})$$

with the usual embeddings $T_1(u) \equiv T(u) \otimes_s \mathbb{1}$ and $T_2(v) \equiv \mathbb{1} \otimes_s T(v)$, where

$$T(u) \equiv \begin{pmatrix} T_1^1(u) & T_2^1(u) \\ T_1^2(u) & T_2^2(u) \end{pmatrix}_{BF} \equiv \begin{pmatrix} A(u) & B(u) \\ C(u) & D(u) \end{pmatrix}_{BF}. \quad (\text{D.4})$$

The PBC SQD is defined as

$$\delta \{T(u)\} \equiv \text{str}_{12} \{ P_{12}^- T_1(u) T_2(u+2\eta) \} \quad (\text{D.5})$$

$$\begin{aligned} &= \frac{1}{2} \{ C(u)B(u+2\eta) - A(u)D(u+2\eta) \\ &\quad - B(u)C(u+2\eta) - D(u)A(u+2\eta) \}. \end{aligned} \quad (\text{D.6})$$

At $v = u + 2\eta$ and after dividing by $a(2\eta)$, the graded YBA yields the commutation relations

$$C(u)B(u+2\eta) - A(u)D(u+2\eta) = C(u+2\eta)B(u) - D(u+2\eta)A(u), \quad (\text{D.7})$$

$$D(u)A(u+2\eta) + B(u)C(u+2\eta) = D(u+2\eta)A(u) - C(u+2\eta)B(u), \quad (\text{D.8})$$

$$B(u)C(u+2\eta) + D(u)A(u+2\eta) = B(u+2\eta)C(u) + A(u+2\eta)D(u). \quad (\text{D.9})$$

These relations can be used to simplify the SQD to

$$\delta \{T(u)\} = -[A(u)D(u+2\eta) - C(u)B(u+2\eta)]. \quad (\text{D.10})$$

It remains to show that the SQD is a central element of the graded YBA, i.e. that it supercommutes with all the other elements $A(v)$, $B(v)$, $C(v)$ and $D(v)$ for arbitrary v . Consider the expression

$$R_{12}(u-v)R_{13}(u-w)R_{23}(v-w)T_1(u)T_2(v)T_3(w). \quad (\text{D.11})$$

Employing the graded YBE once, it is obvious that

$$(\text{D.11}) = R_{23}(v-w)R_{13}(u-w) [R_{12}(u-v)T_1(u)T_2(v)] T_3(w) \quad (\text{D.12})$$

$$\boxed{v \rightarrow u+2\eta} \Rightarrow -2a(2\eta)R_{23}(u-w+2\eta)R_{13}(u-w)P_{12}^-T_1(u)T_2(u+2\eta)T_3(w). \quad (\text{D.13})$$

On the other hand, by applying the graded YBA relation twice, it is found that

$$(\text{D.11}) = T_3(w) [R_{12}(u-v)T_1(u)T_2(v)] R_{13}(u-w)R_{23}(v-w) \quad (\text{D.14})$$

$$\boxed{v \rightarrow u+2\eta} \Rightarrow -2a(2\eta)T_3(w)P_{12}^-T_1(u)T_2(u+2\eta)R_{13}(u-w)R_{23}(u-w+2\eta). \quad (\text{D.15})$$

Equating (D.13) and (D.15) and multiplying from both sides with P_{12}^- gives

$$\begin{aligned} & \{P_{12}^-R_{23}(u-w+2\eta)R_{13}(u-w)P_{12}^-\}\{P_{12}^-T_1(u)T_2(u+2\eta)P_{12}^-\}T_3(w) \\ & = T_3(w)\{P_{12}^-T_1(u)T_2(u+2\eta)P_{12}^-\}\{P_{12}^-R_{13}(u-w)R_{23}(u-w+2\eta)P_{12}^-\}, \end{aligned} \quad (\text{D.16})$$

where additional P_{12}^- projectors have been inserted by virtue of the appropriate triangularity conditions. After a change of basis to the P_{12}^- eigenbasis via A_{12} as defined in (3.14), it is easy to check that application of the supertrace $\text{str}_{12}\{.\}$ yields

$$\sigma_3^z \delta \{T(u)\} T_3(w) = T_3(w) \sigma_3^z \delta \{T(u)\} \quad (\text{D.17})$$

$$\Leftrightarrow [\sigma_3^z \delta \{T(u)\}, T_3(w)] = 0 \quad (\text{D.18})$$

$$\Leftrightarrow [\delta \{T(u)\}, T_j^i(w)]_{\pm} = 0. \quad (\text{D.19})$$

Similarly one may introduce the object

$$\delta\{\hat{T}(u)\} \equiv \text{str}_{12}\{P_{12}^-\hat{T}_2(u)\hat{T}_1(u+2\eta)\} \quad (\text{D.20})$$

which obeys the exact same super commutation relations and by (6.9) turns out to be proportional to the inverse of the above SQD. In particular for the considered N -site small polaron model, it is found that

$$\delta(u) \equiv \delta \{T(u)\} = -\zeta^N(u+2\eta) \prod_{i=1}^N (-\sigma_{q_i}^z), \quad (\text{D.21a})$$

$$\hat{\delta}(u) \equiv \delta\{\hat{T}(u)\} = -\frac{1}{\zeta^N(u)} \prod_{i=1}^N (-\sigma_{q_i}^z), \quad (\text{D.21b})$$

where q_i labels the i th quantum subspace (see section 5.2). Moreover, the commutation relation (D.18) extends to the fused quantities according to

$$[\sigma_{\ll n \gg}^z \delta \{T(u)\}, T_{\ll 1 \dots n \gg}(w)] = 0 \quad (\text{D.22})$$

with $\sigma_{\ll n \gg}^z$ being defined in equation (3.16).

In the open boundary case, the place of $\delta\{T(u)\}$ is taken by another object $\Delta(u)$ which will most appropriately be called the OBC SQD. Generally, the SQD is what you get when you alter the first fusion step such that, instead of creating a *higher dimensional* transfer matrix by projection on a three-dimensional auxiliary space, you now create a *lower dimensional* object by projecting onto the complementary one-dimensional space. In a sense, loosely speaking, you do a reduction instead of a fusion and find that the open boundary SQD factors as follows,

$$\begin{aligned}\Delta(u) &\equiv \text{str}_{12}\{P_{12}K_2^+(u+2\eta)\bar{R}_{12}(-2u-6\eta)K_1^+(u)\mathcal{T}_1^-(u)R_{12}(2u+2\eta)\mathcal{T}_2^-(u+2\eta)\} \\ &= \delta\{K^+(u)\} \cdot \delta\{T(u)\} \cdot \delta\{K^-(u)\} \cdot \delta\{\hat{T}(u)\} \\ &= \left(\frac{\zeta(u+2\eta)}{\zeta(u)}\right)^N \delta\{K^+(u)\} \cdot \delta\{K^-(u)\},\end{aligned}\quad (\text{D.23})$$

where $\mathcal{T}^-(u)$ was defined in (6.8) and

$$\begin{aligned}\delta\{K^+(u)\} &\equiv \text{str}_{12}\{P_{12}^-K_2^+(u+2\eta)\bar{R}_{12}(-2u-3\cdot 2\eta)K_1^+(u)\} \\ &= g(-2u-6\eta) \cdot \det\{K^+(u)\},\end{aligned}\quad (\text{D.24a})$$

$$\begin{aligned}\delta\{K^-(u)\} &\equiv \text{str}_{12}\{P_{12}^-K_1^-(u)R_{21}(2u+2\eta)K_2^-(u+2\eta)\} \\ &= g(2u+2\eta) \cdot \det\{K^-(u+2\eta)\}\end{aligned}\quad (\text{D.24b})$$

with the function $g(u)$ being introduced in the context of (2.5d). Since $\alpha_{\pm} \cdot \beta_{\pm} = 0$, as mentioned in section 6.1, the determinants $\det\{K^{\pm}(u)\}$ depend *only* on the diagonal boundary parameters ψ_{\pm} . This is different from the open XXZ chain, where two parameters for each boundary enter the expression for the quantum determinant.

Appendix E. Transformation matrices

This appendix presents a collection of matrix representations of the various similarity transformations employed in this paper. It is convenient to define the coefficients

$$a_n \equiv \sqrt{\frac{2n}{n+1}} ([n]_q |_{\eta=\eta_n})^{-1/2} \quad \text{and} \quad b = \left(\frac{[2]_q |_{\eta=\eta_2}}{[3]_q |_{\eta=\eta_3}}\right)^{-1/2}, \quad (\text{E.1a})$$

where $[n]_q$ denotes the usual q -deformation of an integer $n \in \mathbb{N}$ defined by

$$[n]_q \equiv \frac{q^n - q^{-n}}{q - q^{-1}} \quad \text{with} \quad q \equiv e^{2i\eta}, \quad (\text{E.1b})$$

and to set

$$A_{(1)} \equiv B_{\ll 1 \gg} \equiv C_{\ll 1 \gg} \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (\text{E.1c})$$

$$A_{(12)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}, \quad (\text{E.2a})$$

$$B_{\ll 12 \gg} = \text{diag}(a_2, 1, a_2) \quad (\text{E.2b})$$

$$C_{\langle\langle 12 \rangle\rangle} = \text{diag}(a_2, 1, 1), \quad (\text{E.2c})$$

$$A_{(123)} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{3}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & \frac{2\sqrt{2}}{3} & -\frac{\sqrt{2}}{3} & 0 & -\frac{\sqrt{2}}{3} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{3} & \frac{2\sqrt{2}}{3} & 0 & -\frac{\sqrt{2}}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{2}}{3} & 0 & -\frac{\sqrt{2}}{3} & -\frac{\sqrt{2}}{3} & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}}{3} & 0 & \frac{2\sqrt{2}}{3} & -\frac{\sqrt{2}}{3} & 0 \end{pmatrix}, \quad (\text{E.3a})$$

$$B_{\langle\langle 123 \rangle\rangle} = \text{diag}(a_3, 1, 1, a_3), \quad (\text{E.3b})$$

$$C_{\langle\langle 123 \rangle\rangle} = \text{diag}(a_3, 1, 1, 1), \quad (\text{E.3c})$$

$$A_{(1234)} =$$

$$\frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 & 0 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{3}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sqrt{2} \\ 0 & \frac{3}{2} & -\frac{1}{2} & 0 & -\frac{1}{2} & 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & \frac{3}{2} & 0 & -\frac{1}{2} & 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{5}{3} & 0 & -\frac{1}{3} & -\frac{1}{3} & 0 & 0 & -\frac{1}{3} & -\frac{1}{3} & 0 & -\frac{1}{3} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & -\frac{1}{2} & 0 & \frac{3}{2} & 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{3} & 0 & \frac{5}{3} & -\frac{1}{3} & 0 & 0 & -\frac{1}{3} & -\frac{1}{3} & 0 & -\frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{3} & 0 & -\frac{1}{3} & \frac{5}{3} & 0 & 0 & -\frac{1}{3} & -\frac{1}{3} & 0 & -\frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{3}{2} & 0 & 0 & 0 & -\frac{1}{2} & 0 & -\frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{3} & 0 & -\frac{1}{3} & -\frac{1}{3} & 0 & 0 & \frac{5}{3} & -\frac{1}{3} & 0 & -\frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{3} & 0 & -\frac{1}{3} & -\frac{1}{3} & 0 & 0 & -\frac{1}{3} & \frac{5}{3} & 0 & -\frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 & \frac{3}{2} & 0 & -\frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 & -\frac{1}{2} & 0 & \frac{3}{2} & -\frac{1}{2} & 0 \end{pmatrix}, \quad (\text{E.4a})$$

$$B_{\langle\langle 1234 \rangle\rangle} = \text{diag}(a_4, 1, b, 1, a_4), \quad (\text{E.4b})$$

$$C_{\langle\langle 1234 \rangle\rangle} = \text{diag}(a_4, 1, b, 1, 1). \quad (\text{E.4c})$$

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