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Non-diagonal boundary conditions for $\mathfrak{gl}(1|1)$ super spin chains

André M Grabinski and Holger Frahm

Institut für Theoretische Physik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany

E-mail: frahm@itp.uni-hannover.de

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Abstract

We study a one-dimensional model of free fermions with $\mathfrak{gl}(1|1)$ supersymmetry and demonstrate how non-diagonal boundary conditions can be incorporated into the framework of the graded quantum inverse scattering method (gQISM) by means of *super matrices* with entries from a superalgebra. For super Hermitian twists and open boundary conditions subject to a certain constraint, we solve the eigenvalue problem for the super transfermatrix by means of the graded algebraic Bethe ansatz technique (gABA) starting from a fermionic coherent state. For generic boundary conditions the algebraic Bethe ansatz cannot be applied. In this case the spectrum of the super transfermatrix is obtained from a functional relation.

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1. Introduction

For a long time studies of quantum integrable models in one spatial dimension have led to important insights into the properties of many-body systems and provided a sound basis for the understanding of the non-perturbative phenomena which arise due to the interplay of interactions and strong quantum fluctuations in low-dimensional systems (see e.g. [1]). A special way to introduce free parameters into these systems is by variation of their boundary conditions. Considering all possible classes compatible with the integrability allows, on one hand, for a complete classification of their low-energy quantum critical behaviour but also to study in detail the effect of embedded impurities and contacts to an environment. Recently, there has been increased interest in twisted or non-diagonal boundary conditions which break certain bulk symmetries of integrable quantum spin chains [2–8]: although their Hamiltonian is a member of a commuting family of operators, the established algebraic schemes for the computation of the spectrum fail unless additional constraints to the boundary conditions are in place. For spin 1/2 chains there has been some progress using functional methods, but

quite a few open questions remain. Even less is known for quantum chains with \mathcal{Z}_2 grading or higher rank symmetry. Although integrable non-diagonal open boundary conditions have been constructed [9–12], the solution of the spectral problem has been restricted to diagonal boundary conditions so far.

In this paper we study this problem for the simplest possible case of spin chains with $\mathfrak{gl}(1|1)$ supersymmetry. Since the corresponding bulk system describes free spinless fermions on a lattice this should provide a toy model to investigate, in particular, the applicability of functional methods to the solution of the spectral problem. We begin with a short review of the graded quantum inverse scattering method [13–15]. Using a Grassmann-valued super matrix representation of the Yang–Baxter algebra, spin chains subject to twisted periodic boundary conditions can be embedded into this framework and are solved exactly. In section 3 we construct the $\mathfrak{gl}(1|1)$ super spin chain with generic open boundary conditions based on Sklyanin’s reflection algebra [16]. We study the spectrum of these super spin chains for certain classes of reflection matrices using the algebraic Bethe ansatz and finally extend this solution to generic boundaries using functional methods.

2. Graded quantum inverse scattering method

The fundamental objects considered within the framework of the graded quantum inverse scattering method (gQISM) are representations $T(v)$ of the *graded Yang–Baxter algebra* (gYBA):

$$R_{12}(u-v) \overset{1}{T}(u) \overset{2}{T}(v) = \overset{2}{T}(v) \overset{1}{T}(u) R_{12}(u-v). \quad (2.1)$$

The indices 1 and 2 label the linear spaces $V_{1,2}$ into which the respective operators are embedded by means of the *super tensor product* \otimes_s , defined through

$$(A \otimes_s B)(C \otimes_s D) \equiv (-1)^{p(B)p(C)} AC \otimes_s BD, \quad (2.2)$$

where $p(X)$ refers to the parity function defined in the appendix. That is, to be precise

$$\overset{1}{T}(u) \equiv T(u) \otimes_s \mathbb{1}, \quad \overset{2}{T}(u) \equiv \mathbb{1} \otimes_s T(u), \quad (2.3)$$

$$R_{12}(u) \equiv R(u) \otimes_s \mathbb{1}, \quad R_{23} \equiv \mathbb{1} \otimes_s R(u) \quad \text{and} \quad R_{13}(u) = P_{23} R_{12}(u) P_{23}.$$

Here P_{ij} is the *graded permutation operator* that interchanges two spaces V_i and V_j according to $P(x \otimes_s y) \equiv (-1)^{p(x)p(y)}(y \otimes_s x)$. The R -matrix is subject to the consistency condition

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

known as the *Yang–Baxter equation* (YBE). As a consequence one obtains local representations $L_{0j}(u) \equiv R_{0j}(u)$ of the gYBA by a graded embedding of the R -matrix. These *Lax-operators* $L_{0j}(u)$ act on an auxiliary space V_0 , whereas their entries act on the j th quantum space V_j . Due to its *comultiplication* property, the gYBA allows for the construction of global representations as products of Lax-operators. This results in a particular representation on the auxiliary space and the tensor product of the quantum spaces $V_q = V_1 \otimes_s V_2 \otimes_s \dots \otimes_s V_N$, the *monodromy matrix*

$$T(u) \equiv L_{0N}(u) L_{0,N-1}(u) \dots L_{01}(u). \quad (2.5)$$

Taking the supertrace (A.11) of this monodromy matrix, we obtain the *super transfermatrix* $\tau(u) = \text{str}\{T(u)\}$ which generates a set of commuting operators on V_q . In particular, it is related to an integrable Hamiltonian with periodic boundary conditions defined by $H = \partial_u \ln \tau(u)|_{u=0}$.

For the $\mathfrak{gl}(1|1)$ supersymmetric representations of the gYBA considered here, this construction leads to a model of free spinless fermions on a one-dimensional lattice with N sites. In the case of periodic boundary conditions the Hamiltonian reads

$$H = \sum_{j=1}^N H_{j,j+1}, \quad H_{j,j+1} \equiv (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) - n_j - n_{j+1} + 1. \quad (2.6)$$

The corresponding R -matrix (cf [15]) is

$$R(u) = \begin{pmatrix} u+1 & & & \\ & u & 1 & \\ & 1 & u & \\ & & & u-1 \end{pmatrix} \curvearrowright \check{R}(u) \equiv P R(u) = \begin{pmatrix} 1+u & & & \\ & 1 & u & \\ & u & 1 & \\ & & & 1-u \end{pmatrix} \quad (2.7)$$

and a graded embedding yields

$$L_{0j}(u) \equiv R_{0j}(u) = \begin{pmatrix} u + e_{j,1}^1 & e_{j,2}^1 \\ e_{j,1}^2 & u - e_{j,2}^2 \end{pmatrix} = \begin{pmatrix} u + \bar{n}_j & c_j^\dagger \\ c_j & u - n_j \end{pmatrix}. \quad (2.8)$$

Generally we will define the Hamiltonian density in terms of the checked R -matrix via $H_{ij} \equiv \partial_u \check{R}_{ij}(u)|_{u=0}$.

2.1. Super Hermitian twists

The simplest generalization of periodic boundary conditions is twists. They can easily be incorporated into the above scheme by making use of the comultiplication property again. Let the *twist matrix* K be a representation of the gYBA on the auxiliary space. Then $K \times T(u)$ is another global representation producing the super transfermatrix

$$\tau(u) = \text{str}\{K \times T(u)\} = \text{str}\{K L_{0N}(u) L_{0,N-1}(u) \dots L_{01}(u)\}, \quad (2.9)$$

which results in a modified Hamiltonian on V_q which contains a boundary term

$$H_{\text{twist}} = \sum_{j=1}^{N-1} H_{j,j+1} + K_N^{-1} H_{N1} K_N. \quad (2.10)$$

As a specific twist matrix we choose

$$K = \begin{pmatrix} a & d\mathcal{E} \\ (d\mathcal{E})^\sharp & b \end{pmatrix} \quad a, b \in \mathbb{R}, \quad d \in \mathbb{C}, \quad (2.11)$$

where \mathcal{E} is the sole generator of $\mathbb{C}\mathcal{G}_1$ (see appendix A.2). Note that this is the most general $\mathbb{C}\mathcal{G}_1$ super matrix being Hermitian with respect to the operation (A.13). Taking into account the properties of Grassmann numbers, K can be diagonalized by a *super unitary* transformation

$$U = \frac{1}{a-b} \begin{pmatrix} i(a-b) & d\mathcal{E}^\sharp \\ d^*\mathcal{E} & i(a-b) \end{pmatrix} \curvearrowright U^\dagger U = U U^\dagger = \mathbb{1}, \quad (2.12)$$

such that

$$\tilde{K} \equiv U^\dagger K U = \begin{pmatrix} a & \\ & b \end{pmatrix}. \quad (2.13)$$

The Lax-operators (2.8) are super matrices over the algebra described in appendix A.1; hence, the comultiplication (2.9) will lead to products between fermionic operators (A.3) and Grassmann numbers. For homogeneous elements $C \in \mathcal{F}$ and $G \in \mathbb{C}\mathcal{G}_N$ we define

$$[C, G]_\pm = 0 \quad \text{and} \quad p(CG) = p(GC) \equiv p(G) + p(C) \pmod{2}. \quad (2.14)$$

In the periodic case (2.6), the spectrum can be obtained by means of the graded algebraic Bethe ansatz (gABA) with the Fock vacuum as a reference state. For diagonal (or upper triangular) twist matrix K the Fock vacuum would still provide a suitable reference state for the gABA. For more general twists a different pseudo-vacuum has to be used.

Using the cyclicity of the supertrace we rewrite the super transfermatrix (2.9) as

$$\tau(u) = \text{str}\{\tilde{K} \tilde{L}_{0N}(u) \tilde{L}_{0,N-1}(u) \dots \tilde{L}_{01}(u)\}, \quad (2.15)$$

with *transformed* Lax-operators

$$\begin{aligned} \tilde{L}_{0j}(u) &\equiv U^\dagger L_{0j}(u) U \\ &= \begin{pmatrix} u + \tilde{n}_j - \frac{d^*}{a-b} \mathcal{E}^\sharp c_j^\dagger + \frac{d}{a-b} \mathcal{E} c_j & c_j^\dagger - \frac{d}{a-b} \mathcal{E} \\ c_j - \frac{d^*}{a-b} \mathcal{E}^\sharp & u - n_j - \frac{d^*}{a-b} \mathcal{E}^\sharp c_j^\dagger + \frac{d}{a-b} \mathcal{E} c_j \end{pmatrix}. \end{aligned} \quad (2.16)$$

By means of a super unitary transformation on the quantum space V_j the Lax-operator $\tilde{L}_{0j}(u)$ can be written in the form (2.8): setting

$$\rho \equiv \frac{d^*}{a-b} \mathcal{E}^\sharp \curvearrowright \rho^\sharp = \frac{d}{a-b} \mathcal{E} \quad (2.17)$$

we define unitary operators

$$Q_j \equiv \mathbb{1} + \rho^\sharp c_j + \rho c_j^\dagger = e^{\rho c_j^\dagger + \rho^\sharp c_j} \curvearrowright Q_j^\dagger \equiv \mathbb{1} - \rho c_j^\dagger - \rho^\sharp c_j = e^{-(\rho c_j^\dagger + \rho^\sharp c_j)} \quad (2.18)$$

that map the fermionic creation and annihilation operators according to

$$\begin{aligned} \tilde{c}_j &= Q_j^\dagger c_j Q_j = c_j - \rho & \text{and} & & \tilde{c}_j^\dagger &= Q_j^\dagger c_j^\dagger Q_j = c_j^\dagger - \rho^\sharp \\ \curvearrowright \tilde{n}_j &\equiv \tilde{c}_j^\dagger \tilde{c}_j = n_j + \rho c_j^\dagger - \rho^\sharp c_j, & \tilde{n}_j &\equiv \tilde{c}_j \tilde{c}_j^\dagger = 1 - \tilde{n}_j = 1 - n_j - \rho c_j^\dagger + \rho^\sharp c_j. \end{aligned} \quad (2.19)$$

In terms of these new fermionic creation and annihilation operators we obtain

$$\tilde{L}_{0j}(u) = \begin{pmatrix} u + \tilde{n}_j & \tilde{c}_j^\dagger \\ \tilde{c}_j & u - \tilde{n}_j \end{pmatrix}. \quad (2.20)$$

After this transformation the gABA can be applied with the new Fock vacuum

$$|\tilde{0}\rangle = e^{-\rho \sum_{j=1}^N c_j^\dagger} |0\rangle \quad (2.21)$$

as the reference state. Note that the local Fock vacua

$$|\tilde{0}_j\rangle = Q_j^\dagger |0_j\rangle = |0_j\rangle - \rho |1_j\rangle \quad (2.22)$$

are *fermionic coherent states*, i.e. eigenstates of the annihilation operator $c_j |\tilde{0}_j\rangle = \rho |\tilde{0}_j\rangle$.

3. Graded reflection algebra

We will now extend Sklyanin's formalism for the treatment of integrable systems with open boundary conditions [16] in a way that makes it applicable to supersymmetric models. Following [17, 18], for a given R -matrix we introduce two associative superalgebras \mathcal{T}_- and \mathcal{T}_+ , subject to the *graded reflection equation*

$$R_{12}(u-v) \overset{1}{\mathcal{T}}_-(u) R_{21}(u+v) \overset{2}{\mathcal{T}}_-(v) = \overset{2}{\mathcal{T}}_-(v) R_{12}(u+v) \overset{1}{\mathcal{T}}_-(u) R_{21}(u-v) \quad (3.1)$$

and to the *dual graded reflection equation*

$$\begin{aligned} R_{21}^{\text{st}_1 \text{ist}_2}(v-u) \overset{1}{\mathcal{T}}_+^{\text{st}_1}(u) \tilde{R}_{12}(-u-v) \overset{2}{\mathcal{T}}_+^{\text{ist}_2}(v) \\ = \overset{2}{\mathcal{T}}_+^{\text{ist}_2}(v) \tilde{R}_{21}(-u-v) \overset{1}{\mathcal{T}}_+^{\text{st}_1}(u) R_{12}^{\text{st}_1 \text{ist}_2}(v-u) \end{aligned} \quad (3.2)$$

respectively, whereas the new matrices \tilde{R} and \bar{R} are related to the R -matrix via

$$\tilde{R}_{12}^{\text{st}_2}(-u-v)R_{21}^{\text{st}_1}(u+v) = \mathbb{1} \quad \text{and} \quad (3.3)$$

$$\bar{R}_{21}^{\text{ist}_1}(-u-v)R_{12}^{\text{ist}_2}(u+v) = \mathbb{1}. \quad (3.4)$$

Moreover the R -matrix (2.7) satisfies the unitarity condition $R_{12}(u-v)R_{21}(v-u) \sim \mathbb{1}$. Under these conditions it is possible to show that the super transfermatrices

$$\tau(u) \equiv \text{str}\{\mathcal{T}_+(u)\mathcal{T}_-(u)\} \quad (3.5)$$

provide a family of commuting operators, i.e. $[\tau(u), \tau(v)] = 0, \forall u, v \in \mathbb{C}$.

Now open boundary conditions can be described by two auxiliary space matrices $K_-(u)$ and $K_+(u)$ satisfying the reflection equations (3.1) and (3.2). Up to normalization, the restriction to $\mathbb{C}G_1$ essentially¹ yields solutions

$$K_{\pm}(u) = \mathbb{1} + u \begin{pmatrix} a_{\pm} & b_{\pm} \mathcal{E} \\ f_{\pm} \mathcal{E}^{\sharp} & -a_{\pm} \end{pmatrix} \quad (3.6)$$

with complex coefficients a_{\pm}, b_{\pm} and f_{\pm} .

Let $T(u)$ be a representation of the gYBA (2.1). Then $T(u)K_-(u)T^{-1}(-u)$ is a further representation of the graded reflection algebra \mathcal{T}_- and we have

$$\tau(u) = \text{str}\{K_+(u)T(u)K_-(u)T^{-1}(-u)\}. \quad (3.7)$$

The R -matrix is regular, that is $R(0) = P$, and for convenience let us choose the normalization such that $K_-(0) = \mathbb{1}$. Since $K_+(0)$ has a vanishing supertrace we compute the second derivative of the super transfermatrix (3.7) and—bearing in mind that the R -matrix (2.7) complies with the unitarity condition only up to normalization—find

$$\left. \frac{d^2}{du^2} \tau(u) \right|_{u=0} = 8[1 + a_+]H \quad (3.8)$$

with the open chain Hamiltonian

$$H = \sum_{j=1}^{N-1} H_{j,j+1} + \frac{1}{2} \left. \frac{d}{du} K_-(u) \right|_{u=0} + \frac{1}{2(1+a_+)} \left. \frac{d}{du} K_+(u) \right|_{u=0}. \quad (3.9)$$

Now we may address the question of what type of boundary terms the matrices K_- and K_+ generate, i.e. in what way such boundary conditions affect the Hamiltonian of the given model. Using the expressions (3.6) explicitly, the Hamiltonian (3.9) can be written as

$$H = \sum_{j=1}^{N-1} H_{j,j+1} + \frac{1}{2} \begin{pmatrix} a_- & d_- \mathcal{E} \\ f_- \mathcal{E}^{\sharp} & -a_- \end{pmatrix}_1 + \frac{1}{2(1+a_+)} \begin{pmatrix} a_+ & d_+ \mathcal{E} \\ f_+ \mathcal{E}^{\sharp} & -a_+ \end{pmatrix}_N. \quad (3.10)$$

In using standard representations of (A.3) and by exploiting (A.14) we can express the two matrices from the latter equation by elements of the combined superalgebra. The first matrix yields

$$\begin{pmatrix} a_- & d_- \mathcal{E} \\ f_- \mathcal{E}^{\sharp} & -a_- \end{pmatrix} = \begin{pmatrix} a_- & \\ & a_- \end{pmatrix} + d_- \begin{pmatrix} 0 & \mathcal{E} \\ 0 & 0 \end{pmatrix} + f_- \begin{pmatrix} 0 & 0 \\ \mathcal{E}^{\sharp} & 0 \end{pmatrix} \quad (3.11)$$

$$= a_- \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + d_- \begin{pmatrix} \mathcal{E} & \\ & -\mathcal{E} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + f_- \begin{pmatrix} \mathcal{E}^{\sharp} & \\ & -\mathcal{E}^{\sharp} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix} \quad (3.12)$$

$$= a_- (\mathbb{1} - 2n) + d_- \mathcal{E} c - f_- \mathcal{E}^{\sharp} c^{\dagger} \quad (3.13)$$

¹ Constant matrices of the form $K_{\pm} = (K_{\pm}(u) - \mathbb{1})/u$ can be employed as well.

and after repeating this procedure for the second matrix, the entire Hamiltonian reads

$$H = \sum_{j=1}^{N-1} H_{j,j+1} + \frac{1}{2} [a_- - 2a_- n_1 + d_- \mathcal{E} c_1 - f_- \mathcal{E}^\# c_1^\dagger] + \frac{1}{2(1+a_+)} [a_+ - 2a_+ n_N + d_+ \mathcal{E} c_N - f_+ \mathcal{E}^\# c_N^\dagger]. \quad (3.14)$$

We point out that the non-diagonal boundary terms, which do not preserve the particle number, are Grassmann valued (i.e. $\sim \mathcal{E}$). Such terms may arise, e.g. in the description of the system coupled to a fermionic environment after integrating out the bath degrees of freedom.

4. Graded algebraic Bethe ansatz

In this section we show how the spectral problem for the Hamiltonian (3.14) can be solved by means of a graded algebraic Bethe ansatz. For notational convenience we set $T(u) \equiv T(u)K_-(u)T^{-1}(-u)$ and consider $T(u)$ as a 2×2 -matrix

$$T(u) \equiv \begin{pmatrix} \mathcal{A}(u) & \mathcal{B}(u) \\ \mathcal{C}(u) & \mathcal{D}(u) \end{pmatrix} \quad (4.1)$$

on the auxiliary space. The reflection equation (3.1) gives commutation relations between the quantum space operators $\mathcal{A}(u)$, $\mathcal{B}(u)$, $\mathcal{C}(u)$ and $\mathcal{D}(u)$ of which the following three are of particular interest:

$$\mathcal{B}(u)\mathcal{B}(v) = \frac{1-u+v}{1+u-v} \mathcal{B}(v)\mathcal{B}(u), \quad (4.2a)$$

$$\mathcal{A}(u)\mathcal{B}(v) = \frac{(1-u+v)(v+u)}{(1+u+v)(v-u)} \mathcal{B}(v)\mathcal{A}(u) + \frac{1}{1+u+v} \mathcal{B}(u) \left\{ \frac{u+v}{u-v} \mathcal{A}(v) - \mathcal{D}(v) \right\}, \quad (4.2b)$$

$$\mathcal{D}(u)\mathcal{B}(v) = \frac{(1-u+v)(v+u)}{(1+u+v)(v-u)} \mathcal{B}(v)\mathcal{D}(u) + \frac{1}{1+u+v} \mathcal{B}(u) \left\{ \frac{u+v}{u-v} \mathcal{D}(v) - \mathcal{A}(v) \right\}. \quad (4.2c)$$

Let $|0\rangle$ be a pseudo-vacuum upon which $T(u)$ acts as an upper triangular matrix, i.e.

$$T(u)|0\rangle = \begin{pmatrix} \mathcal{A}(u)|0\rangle & \mathcal{B}(u)|0\rangle \\ \mathcal{C}(u)|0\rangle & \mathcal{D}(u)|0\rangle \end{pmatrix} = \begin{pmatrix} \alpha(u)|0\rangle & * \neq 0 \\ 0 & \delta(u)|0\rangle \end{pmatrix}. \quad (4.3)$$

Here $\alpha(u)$ and $\delta(u)$ are scalar functions, called *parameters*, that are to be determined later on. They are eigenvalues to $\mathcal{A}(u)$ and $\mathcal{D}(u)$ for the eigenstate $|0\rangle$.

4.1. Diagonal boundary conditions

We begin by considering *diagonal* boundary matrices K_- and K_+ , i.e.

$$K_-(u) = \begin{pmatrix} 1+ua_- & \\ & 1-ua_- \end{pmatrix} \quad \text{and} \quad K_+(u) = \begin{pmatrix} 1+ua_+ & \\ & 1-ua_+ \end{pmatrix}. \quad (4.4)$$

This yields the super transfermatrix

$$\tau(u) = \text{str} \{ K_+(u)T(u) \} = (1+ua_+)\mathcal{A}(u) - (1-ua_+)\mathcal{D}(u). \quad (4.5)$$

Using the commutation relations (4.2a)–(4.2c) we find $\mathcal{B}(v_1) \dots \mathcal{B}(v_M)|0\rangle$ to be an eigenstate of $\tau(u)$ with eigenvalue

$$\Lambda(u) = \left[\prod_{\ell=1}^M \frac{(1-u+v_\ell)(v_\ell+u)}{(1+u+v_\ell)(v_\ell-u)} \right] ((1+ua_+)\alpha(u) - (1-ua_+)\delta(u)), \quad (4.6)$$

provided that the *Bethe ansatz equations*

$$\frac{\alpha(v_j)}{\delta(v_j)} = \frac{1-a_+v_j}{1+a_+v_j} \quad (4.7)$$

are satisfied. Here the functions $\alpha(u)$ and $\delta(u)$ are obtained from the action of $\mathcal{T}(u)$ on the Fock vacuum $|0\rangle$

$$\mathcal{T}(u)|0\rangle = T(u) \overset{0}{K}_-(u) T^{-1}(-u)|0\rangle = \begin{pmatrix} \alpha(u) & \mathcal{B}(u) \\ 0 & \delta(u) \end{pmatrix} |0\rangle. \quad (4.8)$$

Using (2.5) and (2.8) we find

$$\begin{aligned} \alpha(u) &= \left(\frac{1}{1-u^2} \right)^N (1+ua_-)[u+1]^{2N} \\ \delta(u) &= \left(\frac{1}{1-u^2} \right)^N \left\{ (1-ua_-)u^{2N} + (1+ua_-) \frac{u^{2N}}{1+2u} \left(\left[\frac{u+1}{u} \right]^{2N} - 1 \right) \right\}. \end{aligned} \quad (4.9)$$

Therefore, the Bethe ansatz equations

$$\left(\frac{v_j+1}{v_j} \right)^N = \frac{1-a_+v_j}{1+a_+(v_j+1)} \frac{1-a_-(v_j+1)}{1-a_-v_j} \quad (4.10)$$

determine the quantization of single-particle momenta of the free fermions due to the boundary conditions.

Finally, we find an explicit expression for the operators $\mathcal{B}(u)$, that generate eigenstates of the super transfermatrix:

$$\begin{aligned} \mathcal{B}(u) &= \left(\frac{u}{1-u} \right)^N \frac{2}{2u+1} \sum_{\ell=1}^N \left\{ [1+ua_-] \left(\frac{u+1}{u} \right)^{j-1} \right. \\ &\quad \left. + \left[\frac{u}{u+1} - a_- \right] \left(\frac{u}{u+1} \right)^{j-1} \right\} c_\ell^\dagger. \end{aligned} \quad (4.11)$$

4.2. Quasi-diagonal boundary conditions

Application of the graded Bethe ansatz for *non*-diagonal boundary matrices is only possible when a suitable reference state can be found. Here we consider a super Hermitian left boundary matrix K_+

$$K_+(u) = \mathbb{1} + u \begin{pmatrix} a_+ & d_+ \mathcal{E} \\ d_+^* \mathcal{E}^\sharp & -a_+ \end{pmatrix} \quad \text{with} \quad a_+ \in \mathbb{R} \quad \text{and} \quad d_+ \in \mathbb{C}, \quad (4.12)$$

which is diagonalized by the super unitary transformation

$$U = \frac{1}{2a_+} \begin{pmatrix} 2ia_+ & d_+ \mathcal{E}^\sharp \\ d_+^* \mathcal{E} & 2ia_+ \end{pmatrix}, \quad \tilde{K}_+(u) = U^\dagger K_+(u) U = \begin{pmatrix} 1+ua_+ & \\ & 1-ua_+ \end{pmatrix}. \quad (4.13)$$

Now we proceed as in section 2.1: the transformation U leaves the Lax-operators shape-invariant, and we find

$$\tilde{L}_{0j}(u) = U^\dagger L_{0j}(u) U = \begin{pmatrix} u + \tilde{n}_j & \tilde{c}_j^\dagger \\ \tilde{c}_j & u - \tilde{n}_j \end{pmatrix}, \quad (4.14)$$

where $\tilde{c}_j = c_j - \rho$ and $\tilde{c}_j^\dagger = c_j^\dagger - \rho^\sharp$; but now we have

$$\rho \equiv \frac{d_+^*}{2a_+} \mathcal{E}^\sharp \curvearrowright \rho^\sharp = \frac{d_+}{2a_+} \mathcal{E}. \quad (4.15)$$

Due to the cyclicity of the supertrace the super transfermatrix can be written as

$$\tau(u) = \text{str}_0 \{ \overset{\circ}{K}_+(u) \mathcal{T}(u) \} = \text{str}_0 \{ \overset{\circ}{\tilde{K}}_+(u) \tilde{\mathcal{T}}(u) \}, \quad (4.16)$$

where

$$\tilde{\mathcal{T}}(u) = \tilde{T}(u) \overset{\circ}{\tilde{K}}_-(u) \tilde{T}^{-1}(-u) \equiv \begin{pmatrix} \tilde{\mathcal{A}}(u) & \tilde{\mathcal{B}}(u) \\ \tilde{\mathcal{C}}(u) & \tilde{\mathcal{D}}(u) \end{pmatrix}. \quad (4.17)$$

Here we have introduced $\tilde{T}(u) = \tilde{L}_{0N}(u) \dots \tilde{L}_{01}(u)$ and \tilde{K}_- is the transformed right boundary matrix (3.6):

$$\tilde{K}_-(u) = U^\dagger K_-(u) U = \frac{1}{a_+} \begin{pmatrix} a_+(1 + ua_-) & (a_+d_- - d_+a_-)u\mathcal{E} \\ (a_+f_- - d_+^*a_-)u\mathcal{E}^\sharp & a_+(1 - ua_-) \end{pmatrix}. \quad (4.18)$$

Now, choosing the parameters in (4.18) to satisfy the constraint

$$a_+f_- = d_+^*a_-, \quad (4.19)$$

the transformed boundary matrix \tilde{K}_- is upper triangular and the graded algebraic Bethe ansatz can be performed again with a pseudo-vacuum constructed from the fermionic coherent state (2.21) by using definition (4.15) for ρ (see [2] for a similar approach in the ungraded case). Furthermore, since the transformed quantum space operators $\tilde{\mathcal{A}}(u)$, $\tilde{\mathcal{B}}(u)$, $\tilde{\mathcal{C}}(u)$ and $\tilde{\mathcal{D}}(u)$ obey the same fundamental commutation relations (4.2a)–(4.2c) as their original counterparts, the Bethe ansatz equations (4.10) remain unchanged.

Compared to the diagonal case we find that the addition of non-diagonal boundary parameters subject to the constraint (4.19) does not affect the eigenvalues of the super transfermatrix: the energy spectrum of the chain is determined by the diagonal parameters a_\pm of the boundary matrices alone. The Bethe states are generated by the action of the operator $\tilde{\mathcal{B}}$ on the new pseudo-vacuum. Due to the unitary transformation it contains a Grassmann-valued shift

$$\begin{aligned} \tilde{\mathcal{B}}(u) &= \left(\frac{u}{1-u} \right)^N \frac{2}{2u+1} \sum_{\ell=1}^N \left\{ [1 + ua_-] \left(\frac{u+1}{u} \right)^{j-1} \right. \\ &\quad \left. + \left[\frac{u}{u+1} - a_- \right] \left(\frac{u}{u+1} \right)^{j-1} \right\} \tilde{c}_\ell^\dagger + \left(\frac{u}{1-u} \right)^N \left(d_- - \frac{d_+}{a_+} a_- \right) u\mathcal{E}. \end{aligned} \quad (4.20)$$

Therefore, the Bethe states $\tilde{\mathcal{B}}(v_1) \dots \tilde{\mathcal{B}}(v_M) |\tilde{0}\rangle$ are linear combinations of states with up to M particles added to the coherent state Fock vacuum (2.21).

4.3. Generic boundary conditions: functional relations

Finally, we want to address the question to what extent the spectral problem of the $\mathfrak{gl}(1|1)$ -model can be solved if we choose more general boundary matrices than those allowed by the constraint (4.19). In this case a reference state suitable for the application of the gABA is not available.

In the case of spin 1/2 chains without grading this question has been addressed by exploiting certain functional relations obeyed by the eigenvalues of the transfer matrix as a consequence of integrability of the model (see e.g. [3–5, 7]). To obtain such a functional relation for the model considered here we begin with the representation (4.6) of the eigenvalues in terms of roots of the Bethe equations. Note that only the eigenvalues of the boundary matrices enter this expression in the cases studied above.

Let $k_{\pm}^{1,2}$ be the eigenvalues of the boundary matrices $K_{\pm}(u)$, then (4.6) can be rewritten as a functional relation for an unknown function $q(u)$:

$$\Lambda(u) = \frac{q(u-1)}{q(u)} f(u) \tag{4.21}$$

where $f(u)$ is a known function:

$$\begin{aligned} f(u) &\equiv k_+^1 \alpha(u) - k_+^2 \delta(u) \\ &= k_+^1 \left(\frac{1}{1-u^2} \right)^N k_-^1 [u+1]^{2N} \\ &\quad - k_+^2 \left(\frac{u^2}{1-u^2} \right)^N \left\{ k_-^2 + \frac{k_-^1}{1+2u} \left(\left[\frac{u+1}{u} \right]^{2N} - 1 \right) \right\}. \end{aligned} \tag{4.22}$$

By construction $\Lambda(u)$ is a polynomial in u . Therefore, equation (4.21) has to be complemented with the condition that its RHS is analytic. In particular the residues at the zeros of the unknown function $q(u)$ have to vanish. With a polynomial ansatz

$$q(u) \equiv \prod_{\ell=1}^M (-u - 1 - v_{\ell})(u - v_{\ell}), \tag{4.23}$$

this leads immediately to the Bethe equations (4.10).

For spin 1/2 chains it has been observed [5, 7], that the functional equations such as (4.21) hold both in the case of diagonal or quasi-diagonal *and* in the generic off-diagonal boundary conditions: there, only the eigenvalues of the boundary matrices enter the equation explicitly while the deviation from constraints such as (4.19) in the non-diagonal case changes the asymptotic behaviour of its solution. This leads to non-polynomial solutions $q(u)$ to the corresponding difference equations and therefore Bethe-like equations are not easily obtained.

Based on this observation we propose that the eigenvalues of the super transfermatrix (3.7) satisfy equation (4.21) with $f(u)$ parametrized by the eigenvalues of the generic boundary matrices $K_{\pm}(u)$ as in (4.22). We have verified this hypothesis for small system sizes where we are able to explicitly construct the super transfermatrix as a square even super matrix of corresponding finite dimension. Taking into account the peculiarities arising from grading as well as the nilpotency of Grassmann generators, it is perfectly possible to perform an exact diagonalization by the use of computer algebra systems. For chains with up to $N = 6$ sites we have computed the eigenvalues for the most general boundary matrices $K_-(u)$ and $K_+(u)$ and found that the functional equation (4.21) is indeed satisfied. Unlike the situation for spin 1/2 chains, however, the functions $q(u)$ are still polynomial as in (4.23) which allows us to compute the eigenvalues by solving the Bethe equations (4.10) for generic boundary conditions!

As an simple example we consider a system with just one site, i.e. $N = 1$: the exact diagonalization of the corresponding super transfermatrix yields the two eigenvalues

$$\Lambda^\pm(u) = -\frac{2u}{u^2 - 1} (1 + a_+ + u(u \pm 1) [a_+ + a_-(1 + a_+)]). \quad (4.24)$$

On the other hand, assuming that the eigenvalues satisfy (4.21) with polynomial $q(u)$ (4.23) we can determine the values of the parameters v_ℓ from the requirement that $\Lambda(u)$ has vanishing residues at the poles at $u = v_\ell$ and $u = -1 - v_\ell$. For $M = 0$ we immediately obtain $\Lambda^+(u)$ while for $M = 1$ we find

$$v_1 = -\frac{1}{2} \left\{ 1 \pm \sqrt{\frac{a_- + a_+(a_- - 3) - 4}{a_+ + a_-(1 + a_+)}} \right\} \quad (4.25)$$

and thereby recover the second eigenvalue $\Lambda^-(u)$.

5. Summary and conclusion

In this paper we have studied $\mathfrak{gl}(1|1)$ -symmetric super chains of free fermions subject to generic non-diagonal—in general Grassmann-valued—boundary fields breaking the $U(1)$ particle number conservation of the bulk system. The boundary conditions could be embedded into the reflection algebra formalism resulting in quantum integrable models. For the solution of the spectral problem we have applied the graded algebraic Bethe ansatz for a class of boundary conditions satisfying a constraint (4.19). In these cases both the eigenvalues and the eigenstates of the super transfermatrix are obtained by the action of creation operators on a suitably chosen reference state. For generic boundary conditions such a vacuum state could not be constructed. Motivated by recent findings for spin chains without grading, we have proposed the hypothesis that the eigenvalues can still be obtained from Bethe equations and verified this conjecture for small system sizes using numerical methods. In this case, however, it is not clear how the eigenstates are parametrized by the Bethe roots.

Although the case of $\mathfrak{gl}(1|1)$ -symmetric super chains is particular simple since the resulting Hamiltonian describes free particles, our results indicate that it may be easier to deal with non-diagonal boundary fields in integrable super spin chains than in models without grading. A straight forward extension is to the q -deformation of the system presented here. Non-diagonal solutions to the reflection equations for the corresponding small polaron model have been constructed in the past [20, 21]. Studies of the spectral problem for these chains, however, have been restricted to the diagonal case.

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Appendix. Superalgebras and -matrices

A.1. General linear Lie superalgebras

Let $N, m, n \in \mathbb{N}$ and $\{e_{j,\alpha}^\beta\}_{\alpha,\beta=1,\dots,m+n}^{j=1,\dots,N}$ be a homogeneous basis of an associative superalgebra, subject to the commutation relations

$$[e_{j,\alpha}^\beta, e_{k,\gamma}^\delta]_\pm = \delta_{jk} \left(\delta_\gamma^\beta e_{j,\alpha}^\delta - (-1)^{P(e_{j,\alpha}^\beta)P(e_{k,\gamma}^\delta)} \delta_\alpha^\delta e_{j,\gamma}^\beta \right), \quad (A.1)$$

whereas $[X, Y]_{\pm} \equiv XY - (-1)^{p(X)p(Y)}YX$ denotes the so-called *super commutator* and $p(X)$ gives the parity of a homogeneous element X of the superalgebra, that is

$$p(X) = \begin{cases} 0 & \text{if } X \text{ is an element of the even subspace, or} \\ 1 & \text{if } X \text{ is an element of the odd subspace.} \end{cases} \quad (\text{A.2})$$

Considering the super commutator as a generalized Lie product, the generators $e_{j,\alpha}^{\beta}$ constitute the Lie superalgebra $\mathfrak{gl}(m|n)$. We restrict ourselves to the special case $m = n = 1$. By identifying

$$c_j \equiv e_{j,1}^2, \quad c_j^{\dagger} \equiv e_{j,2}^1, \quad n_j \equiv c_j^{\dagger}c_j \equiv e_{j,2}^2 \quad \text{and} \quad \bar{n}_j \equiv c_j c_j^{\dagger} = 1 - n_j \equiv e_{j,1}^1 \quad (\text{A.3})$$

we find $\mathfrak{gl}(1|1)$ to be the algebra \mathcal{F} of operators c_j^{\dagger} and c_j creating and annihilating spinless fermions on a one-dimensional lattice respectively, j being the site index. In this case the even subspace is spanned by n_j and \bar{n}_j , while c_j^{\dagger} and c_j span the odd subspace.

For a more detailed introduction to the construction of superalgebras on graded vector spaces, we refer to [22], [15] and section 12.3 in [1].

A.2. Grassmann algebras

Grassmann numbers, being the elements of a Grassmann algebra, are one of the key ingredients in the formulation of non-diagonal boundary conditions for super spin chains. The $\mathcal{N} \in \mathbb{N}$ generators of a Grassmann algebra will be denoted by $\mathcal{E}_1, \mathcal{E}_2, \dots, \mathcal{E}_{\mathcal{N}}$ and in accordance with [22] we define a product between them such that for all $j, k, l = 1, 2, \dots, \mathcal{N}$

(i) the product is associative,

$$(\mathcal{E}_j \mathcal{E}_k) \mathcal{E}_l = \mathcal{E}_j (\mathcal{E}_k \mathcal{E}_l), \quad (\text{A.4})$$

(ii) any two generators mutually anticommute,

$$\mathcal{E}_j \mathcal{E}_k = -\mathcal{E}_k \mathcal{E}_j, \quad (\text{A.5})$$

(iii) and each non-zero product

$$\mathcal{E}_{j_1} \mathcal{E}_{j_2} \dots \mathcal{E}_{j_r}, \quad 1 \leq r \leq \mathcal{N} \quad (\text{A.6})$$

involving r generators is linearly independent of products involving less than r generators.

In particular, this means that Grassmann generators \mathcal{E}_j have *no inverse*.

For consistency reasons it is customary to supplement the set of generators by an identity 1 with the defining properties $1 \times 1 = 1$ and $1\mathcal{E}_j = \mathcal{E}_j 1 = \mathcal{E}_j$. Using multi-index notation, each product of $|\mu|$ generators can be written as $\mathcal{E}_{\mu} \equiv \mathcal{E}_{j_1} \mathcal{E}_{j_2} \dots \mathcal{E}_{j_{|\mu|}}$, whereas $\mu = \{j_1, j_2, \dots, j_{|\mu|}\}$ is an, without loss of generality, ascendingly ordered set of natural numbers $1 \leq j_n \leq \mathcal{N}$. The identity may be incorporated by setting $\mathcal{E}_{\emptyset} \equiv 1$. Finally, this enables us to express every Grassmann number G as a linear combination of generator products \mathcal{E}_{μ} with complex coefficients G^{μ} :

$$G = \sum_{\mu} G^{\mu} \mathcal{E}_{\mu}. \quad (\text{A.7})$$

Here the summation is to be carried out over all multi-indices μ . In the following text this complex Grassmann algebra with \mathcal{N} generators will be labelled $\mathbb{C}G_{\mathcal{N}}$. We impose a convenient grading, setting

$$p(\mathcal{E}_{\mu}) \equiv |\mu| \pmod{2}. \quad (\text{A.8})$$

The complex conjugation of a Grassmann number G is given by the complex conjugation of the linear coefficients in (A.7), i.e. $G^* \equiv (G^{\mu})^* \mathcal{E}_{\mu}$. Moreover, we define the adjoint G^{\sharp} of a Grassmann number G by

$$G^{\sharp} \equiv (-i)^{p(\mathcal{E}_{\mu})} (G^{\mu})^* \mathcal{E}_{\mu}. \quad (\text{A.9})$$

A.3. Super matrices

Just like the elements of the above superalgebras, super matrices are graded objects. Here we will only make use of square *even* invertible super matrices M , having the partitioning

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \quad (\text{A.10})$$

such that all entries of the submatrices A and D are *even* elements of a superalgebra, whereas all entries of the submatrices B and C are *odd* elements of the same superalgebra. We define convenient analogs to the usual matrix operations. The *supertrace* is given by

$$\text{str} \{M\} \equiv \text{tr} \{A\} - \text{tr} \{D\}. \quad (\text{A.11})$$

In contrast to the ordinary matrix transposition, the *super transposition* $()^{\text{st}}$ is not an involution. Therefore, we have an additional *inverse super transposition* $()^{\text{ist}}$:

$$M^{\text{st}} \equiv \begin{pmatrix} A^T & C^T \\ -B^T & D^T \end{pmatrix}, \quad M^{\text{ist}} \equiv \begin{pmatrix} A^T & -C^T \\ B^T & D^T \end{pmatrix}. \quad (\text{A.12})$$

If the underlying superalgebra is $\mathbb{C}G_{\mathcal{N}}$ there are two more important operations, namely the *adjoint* operation

$$M^{\dagger} \equiv \begin{pmatrix} (A^{\sharp})^T & (C^{\sharp})^T \\ (B^{\sharp})^T & (D^{\sharp})^T \end{pmatrix}, \quad (\text{A.13})$$

where A^{\sharp} is defined by entrywise application of (A.9), and the multiplication of a super matrix by a Grassmann number G of definite parity:

$$G \cdot M \equiv \begin{pmatrix} G \mathbb{1}_{\dim A} & 0 \\ 0 & (-1)^{p(G)} G \mathbb{1}_{\dim D} \end{pmatrix} \begin{pmatrix} A & B \\ C & D \end{pmatrix}. \quad (\text{A.14})$$

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