Bethe ansatz solution of the small polaron with nondiagonal boundary terms

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Abstract. The small polaron with generic, nondiagonal boundary terms is
investigated within the framework of quantum integrability. The fusion hierarchy
of the transfer matrices and its truncation for particular values of the anisotropy
parameter are both employed, so that the spectral problem is formulated in terms
of a TQ equation. The solution of this equation for generic boundary conditions
is based on a deformation of the diagonal case. The eigenvalues of the model are
extracted and the corresponding Bethe ansatz equations are presented. Finally, we
comment on the eigenvectors of the model and explicitly compute the eigenstate
of the model which evolves into the Fock vacuum when the off-diagonal boundary
terms are switched off.

Keywords: integrable spin chains (vertex models), quantum integrability (Bethe
ansatz), solvable lattice models

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1. Introduction

The investigation of exactly solvable models over many years has proved to be very fruitful in extracting physical information regarding phenomena lying in strongly coupled regimes [1]. For integrable models in one spatial dimension, the framework of the quantum inverse scattering method (QISM) [2, 3] provides an efficient way of computing the various physical quantities. In this paper we study the small polaron model, which can also be regarded as a graded version of the XXZ quantum spin chain. The $R$-matrix satisfies the graded Yang–Baxter equation [4]–[6]

\[ R_{12}(\lambda) R_{13}(\lambda + \mu) R_{23}(\mu) = R_{23}(\mu) R_{13}(\lambda + \mu) R_{12}(\lambda), \]

and the resulting bulk Hamiltonian coincides with the bulk Hamiltonian of the XXZ spin chain, after employing a Jordan–Wigner transformation. The effects of supersymmetry become visible when periodicity of the boundary conditions is relaxed; hence more general boundaries are considered, corresponding to open boundaries in the spin chain picture.

Within a graded version of Sklyanin’s reflection algebra [7] these boundary conditions can be implemented while keeping the integrability of the model. For purely diagonal boundary fields, i.e. respecting the $U(1)$ symmetry of the bulk, the spectrum of the model can be obtained using algebraic Bethe ansatz (ABA) methods. For nondiagonal boundary conditions, however, this symmetry is broken and a simple reference state does not exist anymore, rendering the ABA framework insufficient.

For the respective ungraded model various methods have been successfully employed in the past, such as the fusion hierarchy of the transfer matrices and its truncation [9, 10], the construction of a vacuum state by using gauge transformations [11], and generalized TQ equations [12]. All of these approaches, however, rely on the boundary parameters.
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satisfying certain algebraic relations or are restricted to particular values of the bulk anisotropy parameter. No such constraints on the system parameters appear in solutions using the representation theory of the $q$-Onsager algebra [13], in terms of functional relations derived directly from the Yang–Baxter algebra [14], or by separation of variables [15]–[17]. So far, an actual solution of the eigenvalue problem in these formulations is possible for relatively small systems only and it is unclear how the thermodynamic limit can be approached.

Motivated by a recent analysis of the free fermion case [18] where the Grassmannian nature of the nondiagonal boundary parameters was proven sufficient to solve the model without imposing any constraints, we studied the small polaron model with nondiagonal boundary conditions, expecting that a similar situation may also hold. As will become transparent in the following sections, it turns out that this is the case for the interacting fermions as well: supersymmetry lifts the need to impose constraints on the boundary parameters. Furthermore, the structure of the eigenvectors is greatly restricted, so that certain eigenstates can be computed exactly for an arbitrary number of chain sites.

The paper is organized as follows. First, we describe the basic facts of the small polaron model and set up our conventions. In section 3 we first recall the functional equations relating the commuting transfer matrices obtained within the fusion approach obtained in [19]. Based on these findings we proceed to derive higher order functional equations for the transfer matrix of the small polaron model for particular values of the anisotropy parameter which can be formulated as a vanishing determinant condition. The latter allows the spectral problem to be formulated in terms of a TQ equation. Based on the comparison with a particular limit of the fusion hierarchy we conjecture that this equation actually describes the spectrum of the model without any restrictions on the system parameters, i.e. anisotropy and boundary fields. This is supported by the fact that the solution for diagonal boundary conditions can be shown to be equivalent to what has been found previously using algebraic or coordinate Bethe ansatz methods. In section 4 we proceed with solving the full nondiagonal model, by deforming the corresponding problem of the diagonal case. The transfer matrix eigenvalues are found to depend on two distinct sets of Bethe roots, which satisfy two coupled sets of Bethe ansatz equations (BAEs). In section 5 we compute the ‘vacuum eigenstate’ of the model, i.e. the unique state which reduces to the Fock vacuum in the limit of diagonal boundary fields. Based on this result we propose an expression for the generic structure of the eigenvectors of the model which allows for a complete solution of the spectral problem in principle. We conclude by discussing our results and future directions.

2. The small polaron with open boundary conditions

The small polaron model [20, 21] describes the motion of an additional electron in a polar crystal. The physics of these interactions is captured by the following bulk Hamiltonian:

$$H_{\text{bulk}} = \sum_{j=1}^{N-1} -t(c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1}) + V(n_{j+1} n_j + \bar{n}_{j+1} \bar{n}_j), \quad (2.1)$$

where $c_{j+1}^\dagger$ and $c_j^\dagger$ denote the creation and annihilation operators of spinless fermions at site $k$ respectively, obeying anticommutation relations $\{c_k^\dagger, c_l\} = \delta_{kl}$. We have also introduced
the occupation number operators \( n_k = c_k^\dagger c_k \) and \( \bar{n}_k = 1 - n_k \), so that the parameters \( t \) and \( V \) may be interpreted as the hopping amplitude and density–density interaction strength respectively. It is possible to derive the above Hamiltonian through the QISM framework, thus rendering the system integrable [22]. In the Hamiltonian (2.1), periodic boundary conditions are to be assumed. However, periodicity can be relaxed and one may consider integrable open boundary conditions, by using the framework of quantum integrability for models with open boundaries [7]. The full Hamiltonian of the system contains the additional boundary terms, which in general may be nondiagonal ones

\[
H = H_{\text{bulk}} + H_{\text{diag}} + H_{\text{nondiag}}.
\]

Since we deal with a fermionic lattice model, the local space of states is \( \mathbb{Z}_2 \)-graded [24]. The tensor product is graded according to the rule

\[
(A \otimes_B)^{ac}_{bd} = (-1)^{p(a) + p(b) + p(c)} A^a_b B^c_d,
\]

where the parity \( p(a) \) is equal to zero (one) for bosonic (fermionic) indices. All matrix operations below, such as the super trace of a matrix, are then to be understood as operations on super matrices. We omit the definitions of these matrix operations and refer the interested reader to the references [23, 24], whose conventions we follow. The fundamental super transfer matrix of the model is given by the super trace

\[
t(u) = \text{str}_0 \{ K^+(u) T(u) K^-(u) \hat{T}(u) \},
\]

where the monodromy matrices are defined as

\[
T(u) = R_{N0}(u) \cdots R_{20}(u) R_{10}(u), \quad \hat{T}(u) = R_{01}(u) R_{02}(u) \cdots R_{0N}(u).
\]

The \( R \)-matrix is given by

\[
R_{ij}(u) = \frac{1}{\sin(2\eta)} \begin{pmatrix}
\sin(u + 2\eta) & 0 & 0 & 0 \\
0 & \sin(u) & \sin(2\eta) & 0 \\
0 & \sin(2\eta) & \sin(u) & 0 \\
0 & 0 & 0 & -\sin(u + 2\eta)
\end{pmatrix},
\]

acting on the tensor product \( V_i \otimes V_j \) of two linear spaces \( \sim \mathbb{C}^2 \). It satisfies the graded Yang–Baxter equation (1.1) and enjoys several useful properties, such as unitarity

\[
R_{12}(u) R_{21}(-u) = \zeta(u),
\]

crossing symmetry

\[
R_{21}^{st2}(-u - 4\eta) R_{21}^{st1}(u) = \zeta(u + 2\eta),
\]

and periodicity

\[
R_{12}(u + \pi) = -\sigma^z_{12}(u) \sigma^z_1 = -\sigma^z_{12}(u) \sigma^z_2.
\]

In the above we have also defined

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

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The $K$-matrices, which contain the boundary information, satisfy the graded reflection algebra [7, 8] and have the following generic expressions (see also [25]–[27]):

\[
K^-(u) = \omega^- \begin{pmatrix} 
\sin(u + \psi^-) & \alpha^- \sin(2u) \\
\beta^- \sin(2u) & -\sin(u - \psi^-)
\end{pmatrix},
\]

\[
K^+(u) = \omega^+ \begin{pmatrix} 
\sin(u + 2\eta + \psi^+) & \alpha^+ \sin(2u + 4\eta) \\
\beta^+ \sin(2u + 4\eta) & \sin(u + 2\eta - \psi^+)
\end{pmatrix},
\]

with normalizations $\omega^\pm$ defined by

\[
\omega^- \equiv \frac{1}{\sin \psi^-} \quad \text{and} \quad \omega^+ \equiv \frac{1}{2 \cos 2\eta \sin \psi^+}.
\]

The boundary parameters $\psi^\pm$ are commuting numbers with a non-vanishing complex part, while the parameters $\alpha^\pm, \beta^\pm$ are odd Grassmann numbers and anticommute,

\[
[\psi^+, \psi^-] = 0 = \{\alpha^\pm, \alpha^\pm\} = \{\beta^\pm, \beta^\pm\} = \{\beta^\pm, \beta^\pm\}.
\]

Moreover, the reflection algebra is only satisfied provided that the odd Grassmann numbers are subject to the condition $\alpha^+ \cdot \beta^+ = 0 = \alpha^- \cdot \beta^-$.

The bulk part of this Hamiltonian coincides with the expression (2.1) after identifying $t = -\csc 2\eta$ and $V = \cot 2\eta$. The boundary terms obtained with (2.11) read as

\[
H_{\text{diag}} = N_+ \tilde{n}_N - N_- n_N + \frac{1}{2} \cot \psi^- (\tilde{n}_1 - n_1)
\]

\[
H_{\text{nondiag}} = \csc \psi^- (\alpha^- c_1 - \beta^- c_1^\dagger) + \csc \psi^+ (\alpha^+ c_N - \beta^+ c_N^\dagger),
\]

where the following shorthand has been also introduced: $N_\pm \equiv \frac{1}{2} \csc(2\eta) \csc(\psi_\pm) \sin(2\eta \pm \psi_\pm)$. The diagonal boundary terms can be identified with the static boundary chemical potentials at the first and last sites of the lattice, respectively. By means of a Jordan–Wigner transformation the bulk and diagonal boundary terms can be mapped to a spin-1/2 XXZ Heisenberg chain with boundary magnetic fields, see also appendix. This is not possible for the off-diagonal terms breaking the $U(1)$ symmetry of the system. In the small polaron formulation the terms in $H_{\text{nondiag}}$ can be interpreted as sources and sinks for injection of additional particles into the system. Their amplitudes are odd Grassmann numbers, reflecting the fermionic nature of the corresponding reservoir. The Jordan–Wigner transformation of these terms yields a non-local expression in the spin chain formulation.

The super transfer matrix enjoys crossing symmetry

\[
t(-u - 2\eta) = t(u),
\]

and periodicity

\[
t(u + \pi) = t(u).
\]
For future use, we also note that the open transfer matrix is normalized as \( t(0) = 1 \) and becomes diagonal in the semi-classical limit \( \eta \to 0 \),

\[
t(u)|_{\eta=0} = \frac{(\sin u)^{2N}}{\sin \psi_+ \sin \psi_-} \left[ 2\sin^2 u \cos^2 u (\beta^+ \alpha^- - \alpha^+ \beta^-) \prod_{k=1}^{N} \sigma_k^z \right.
\]
\[
- (\cos^2 u \sin \psi_- \sin \psi_+ + \sin^2 u \cos \psi_- \cos \psi_+) \mathbb{1} \].
\]

Finally, taking the limit \( z \equiv e^{iu} \to \infty \), the asymptotic behavior of the super transfer matrix is obtained, which is needed for later comparison. The leading term contains only odd Grassmann boundary parameters and has the expression

\[
t(z) = \left( \frac{z}{2i \sin 2\eta} \right)^{2N} \left( \frac{\omega^+ \omega^-}{4} e^{4\eta (\beta^+ \alpha^- - \alpha^+ \beta^-)} \right).
\]

This particular combination of the odd Grassmann boundary parameters emerges in many different relations, and as will become transparent below it appears uniquely in all eigenvalues of the transfer matrix; thus, henceforth it will be denoted as

\[
G \equiv \beta^+ \alpha^- - \alpha^+ \beta^-.
\]

### 3. Functional relations

As stated in the introduction our analysis of the spectral problem for the transfer matrix of the small polaron model relies on its reformulation in terms of functional equations. To keep the presentation of our results self-contained we begin by recalling the results of [19], namely the infinite hierarchy of fused transfer matrices and its truncation for particular values of the anisotropy parameter \( \eta \). Then we use the truncation identity to rewrite the fusion hierarchy as a higher order functional relation for the transfer matrix (2.4) alone. This relation is then shown to be equivalent to a vanishing determinant condition which allows for the formulation of the spectral problem in terms of a TQ equation. We then argue that this TQ equation holds for arbitrary values of the anisotropy and generic nondiagonal boundary conditions.

#### 3.1. Fusion hierarchy and truncation identities

Having a transfer matrix at hand, one may construct a family of commuting transfer matrices derived from auxiliary spaces of higher dimension through a fusion procedure [31, 32]. Choosing a suitable normalization, the fused transfer matrices form a hierarchy related by the recursion relations

\[
t^{(n)}(u) \cdot t^{(1)}(u + n \cdot 2\eta) = t^{(n+1)}(u) - \tilde{\Delta}(u + [n - 1] \cdot 2\eta) \cdot t^{(n-1)}(u)
\]
with \( t^{(0)} \equiv 1 \) and \( t^{(1)} \equiv -t(u) \). The function \( \tilde{\Delta}(u) \) is up to a scaling factor the super quantum determinant of the small polaron model \[19\]
\[
\tilde{\Delta}(u) \zeta(2u + 4\eta) \equiv \Delta(u) = \zeta^{2N}(u + 2\eta)g(-2u - 6\eta)g(2u + 2\eta) \det K^+(u) \det K^-(u + 2\eta).
\]
(3.2)
Note that the quantum determinant does not depend on the off-diagonal elements of the boundary matrices \( K^{\pm}(u) \) as a consequence of the nilpotency of the odd Grassmann parameters. Since the fused transfer matrices commute with each other, the fusion hierarchy can be also read as a set of relations between their eigenvalues, which after shifting the spectral parameter \( u \to u - n \cdot 2\eta \) gives
\[
- \Lambda(u) = \frac{\Lambda^{(n+1)}(u - n \cdot 2\eta)}{\Lambda^{(n)}(u - n \cdot 2\eta)} - \tilde{\Delta}(u - 2\eta) \frac{\Lambda^{(n-1)}(u - n \cdot 2\eta)}{\Lambda^{(n)}(u - n \cdot 2\eta)}.
\]
(3.3)
For later use we rewrite these equations in terms of the functions
\[
\Lambda^{(n)}(u - n \cdot 2\eta) \equiv Q^{(n)}(u) \prod_{k=0}^{n} \kappa(u - k \cdot 2\eta),
\]
(3.4)
giving
\[
- \Lambda(u) = h^+(u) \frac{Q^{(n+1)}(u + 2\eta)}{Q^{(n)}(u)} - h^-(u) \frac{Q^{(n-1)}(u - 2\eta)}{Q^{(n)}(u)},
\]
(3.5)
h^+(u) = \kappa(u + 2\eta), \quad h^-(u) = \tilde{\Delta}(u - 2\eta) \frac{1}{\kappa(u)}.
Note that while the coefficient functions \( h^\pm(u) \) can be modified by choosing different factors \( \kappa(u) \) in the definition of \( Q^{(n)}(u) \) they always factorize the rescaled quantum determinant, i.e. \( h^+(u)h^-(u + 2\eta) = \tilde{\Delta}(u) \).

The functional equations (3.3) constitute a set of relations for an infinite set of unknown functions \( \tilde{\Lambda}^{(n)}(u) \). Restricting the anisotropy parameter to ‘roots of unity’, \( \eta_n = ((\pi/2)/(n + 1)) \), it has been shown that the fused transfer matrices at levels \( n + 1 \) and \( n - 1 \) are related by the truncation identity \[19\]
\[
t^{(n+1)}(u, \eta_n) = \phi^\text{id}_n(u) \cdot \mathbb{I} - \phi^\text{\tilde{\Delta}}_n(u) \cdot t^{(n-1)}(u + 2\eta_n, \eta_n),
\]
(3.6)
where the functions \( \phi^\text{id}_n(u), \phi^\text{\tilde{\Delta}}_n(u) \) are given by the following expressions:
\[
\phi^\text{id}_n(u) = \mathcal{M}^N_n(u) \mu^+_n(u) \mu^-_n(u) [\nu^+_n(-u)\nu^-_n(u) + \nu^+_n(u)\nu^-_n(-u)],
\]
(3.7)
\[
\phi^\text{\tilde{\Delta}}_n(u) = \zeta^{2N}(u) \mu^+_n(u) \mu^-_n(u),
\]
with
\[
\mathcal{M}_n(u) \equiv \left( \frac{1/2}{\sin 2\eta_n} \right)^n \frac{\sin([n + 1]u)}{\sin 2\eta_n},
\]
\[
\mu^+_n(u) \equiv \pm \delta \{ K^\pm(u - 2\eta_n, \eta_n) \} \frac{\sin(2\eta_n)}{\sin(2u - 2\eta_n)} \prod_{k=2}^{2n} \frac{\sin(2u + k \cdot 2\eta_n)}{\sin(2\eta_n)},
\]
(3.8)
\[
\nu^+_n(u) \equiv \mp \frac{\omega^+_n(u)}{\mu^+_n(u)} \left( \frac{\omega^+_n(u)}{2} \right)^n \frac{\sin([n + 1][u \pm \psi]_n)}{\sin(2\eta_n)} \prod_{i=1}^{n} \prod_{j=1}^{i} \frac{\sin(2u + [i + j] \cdot 2\eta_n)}{\sin(2\eta_n)}.
\]

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3.2. Higher order functional equation and determinant representation

Combining the fusion hierarchy with the truncation identity for a particular value \( n \) yields an \( (n + 1) \)-order functional equation for the transfer matrix of the model with the corresponding anisotropy \( \eta = \eta_n \). Unfortunately, it does not seem possible to write the functional relations in a closed form. Starting from low values of \( n \), one observes that at each level new terms emerge and their number is given by the Fibonacci numbers \( F(n) \). In particular, at a given value \( n \), there are

\[
F(n + 1) + F(n - 1) + 1, \quad n = 2, 3, \ldots
\]

terms in total. Nevertheless, after carefully examining the structure of the functional relations, it is seen that the following simple schematic structure appears:

\[
t(u) t(u + 2\eta) \cdots t(u + (2n - 2)\eta) + \mathcal{O}_n + \phi_{n-1}^\tau(u) \cdot \mathcal{O}_0 = \phi_{n-1}^\text{id}(u) + \prod_{k=0}^{(n/2)-1} \tilde{\Delta}(u + 4k\eta) + \phi_{n-1}^\tau(u) \prod_{k=1}^{(n/2)-1} \Delta(u + (4k - 2)\eta). \tag{3.9}
\]

First, we should note that the last two terms on the RHS are present only for even values of \( n \). Next, the symbol \( \mathcal{O} \) stands for the following sequence:

\[
\mathcal{O}_1 := \sum_{q_0=0}^{n-2} \tilde{\Delta}(u + 2q_0\eta) \mathcal{T}_{q_0}(u)
\]

\[
+ \sum_{q_1=0}^{n-4} \tilde{\Delta}(u + (2q_1 + 4)\eta) \sum_{q_0=0}^{q_1} \tilde{\Delta}(u + 2q_0\eta) \mathcal{T}_{q_0,q_1}(u)
\]

\[
+ \sum_{q_2=0}^{n-6} \tilde{\Delta}(u + (2q_2 + 8)\eta) \sum_{q_1=0}^{q_2} \tilde{\Delta}(u + (2q_1 + 4)\eta) \sum_{q_0=0}^{q_1} \tilde{\Delta}(u + 2q_0\eta) \mathcal{T}_{q_0,q_1,q_2}(u)
\]

\[
+ \cdots, \tag{3.10}
\]

with

\[
\mathcal{T}_{q_0,q_1,\ldots,q_l}(u) = \prod_{m=0}^{n-1} t(u + 2mn\eta), \quad \mathcal{Q} = \bigcup_{k=1}^{l} \{ q_k + 2k; q_k + 2k + 1 \}.
\]

A similar structure holds for \( \mathcal{O}_0 \) as well, although some lower/upper limits of the sums and the product are different. Nevertheless, the structure above is reminiscent of a path-ordered exponential, and appears as some deformed discrete version of the latter one. It would be interesting to see whether this observation possesses some physical meaning, i.e., whether the corresponding operator in the path-ordered exponential plays some physical role here.

Despite the fact that the functional relations cannot be written in a closed form, they can be cast into a vanishing determinant representation as a consequence of the restriction \( m \not\in \mathcal{Q} \) in equation (3.10) above. This leads to the derivation of a TQ equation for the eigenvalues of the transfer matrix (2.4) \[34\]. For the small polaron model, it turns out that the vanishing determinant representation has the same structure as the corresponding one of the XXZ model \[10\]. In particular, the functional relations (3.9) can also be written in
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from (3.11) to be identical. This gives

\[ h(u + 2\eta) \tilde{h}(u - 2\eta) = -\tilde{\Delta}(u), \]

\[ h(u) \tilde{h}(u + 2(n - 1)\eta) = -\phi_n^+(u), \]

\[ \prod_{k=0}^{n} h(u + 2k\eta) + \prod_{k=-1}^{n-1} \tilde{h}(u + 2k\eta) = \phi_n^{id}(u). \]  

(3.12)

Inspired by the structure of the \( h \)-functions in the XXZ case [10], as well as the functions found in [19], we consider the following expressions:

\[ \tilde{h}(u) = h(-u - 4\eta), \quad h(u) = \left( \frac{\sin(u + 2\eta)}{\sin 2\eta} \right)^{2N} \frac{\sin(2u + 4\eta)}{\sin(2u + 2\eta)} g_-(u)g_+(u), \]  

(3.13)

where the boundary information is contained in the functions \( g_\pm(u) \). Substituting the above expressions into (3.12), the following condition arises regarding the functions \( g_\pm(u) \):

\[ g_-(u + 2\eta)g_-(u - 2\eta)g_+(u + 2\eta)g_+(u - 2\eta) = -\det K^+(u) \det K^-(u + 2\eta). \]  

(3.14)

Assuming that the functions \( g_\pm(u) \) factorize the determinants of the reflection matrices and recalling the explicit expressions for the determinants of the boundary matrices, one obtains

\[ g_-(u)g_-(u) = \det K_-(u) = -(\omega^-)^2 \sin(u + \psi_-) \sin(u - \psi_-) \]

\[ g_+(u)g_+(u) = -\det K^+(u - 2\eta) = -(\omega^+)^2 \sin(u + \psi_+) \sin(u - \psi_+), \]  

(3.15)

pinpointing the natural solutions

\[ g_-(u) = \omega^- \sin(u + \psi_-), \quad g_+(u) = \omega^+ \sin(u + \psi_+). \]  

(3.16)

Using the expressions (3.13) and (3.16) then, it is straightforward to check that all three relations in (3.12) are automatically satisfied, so that the expressions for \( h(u), \tilde{h}(u) \) are now proven. It is interesting to point out that the structure we have found here is identical to the corresponding structure of the purely diagonal XXZ case [10].

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The vanishing determinant guarantees the existence of a nontrivial null vector, $(Q_0, Q_1, \ldots, Q_n)$, so that the following relations hold:

\[
\begin{align*}
\Lambda_0 Q_0 - \Lambda_{-1} Q_1 - h_0 Q_n &= 0, \\
-\Lambda_k Q_k - \Lambda_{k-1} Q_{k+1} - \Lambda_{k-1} Q_0 - \Lambda_n Q_{n-1} &= 0, \quad k = 1, \ldots, n - 1, \\
-\Lambda_{n-1} Q_0 - h_n Q_{n-1} + \Lambda_n Q_n &= 0.
\end{align*}
\]

(3.17)

For the present choice of the quasi-classical parameter, i.e. $\eta = \eta_n = (\pi/2)/(n + 1)$, these equations can be recast as TQ equations for a periodic function $Q(u) = Q(u + \pi)$ by identifying $Q_k \equiv Q(u + 2\eta k)$,

\[
\Lambda(u) = h(u) \frac{Q(u - 2\eta) - Q(u + 2\eta)}{Q(u), \quad \text{for } \eta = \eta_n.
\]

(3.18)

Here the degree of the Fourier polynomial for the function $Q(u)$ depends on the choice of the anisotropy $\eta = \eta_n$ (or, equivalently, the level of the fusion hierarchy where the truncation identity (3.6) appears). We note that as a consequence of equations (2.16) and (3.18) the function $Q(u)$ is crossing symmetric.

We emphasize that up to this point we have made no assumptions concerning the form of the reflection matrices $K^\pm(u)$. In particular, the functional equation (3.18) holds for both diagonal and non-diagonal boundary conditions and coincides with the limit $n \to \infty$ of equation (3.5) of the fusion hierarchy provided that the limit $\lim_{n \to \infty} Q^{(n)}(u) = Q(u)$ exists [33]. The first of the conditions (3.12) used to derive the determinant representation of the functional equation guarantees the factorization $h^+(u)h^-(u + 2\eta) = -h(u + 2\eta)h(-u - 2\eta) = \check{\Delta}(u)$ of the quantum determinant with

\[
h^-(u) = -h^+(-u - 2\eta)
\]

\[
= -\omega^+\omega^- \left( \frac{\sin(u + 2\eta)}{\sin 2\eta} \right)^{2N} \frac{\sin(2u + 4\eta)}{\sin(2u + 2\eta)} \sin(u + \psi_+) \sin(u + \psi_-),
\]

(3.19)

corresponding to

\[
\kappa(u) = \omega^- \omega^+ \left( -\frac{\sin(u - 2\eta)}{\sin 2\eta} \right)^{2N} \frac{\sin(2u - 4\eta)}{\sin(2u - 2\eta)} \sin(u - \psi_) \sin(u - \psi_+),
\]

(3.20)
in the definition of the $Q^{(n)}(u)$.

For the limit $\lim_{n \to \infty} Q^{(n)}(u)$ to exist, however, this choice of the function $h(u)$ is not sufficient for general boundary conditions: in section 4 we shall introduce deformations of the functions $h$ and $Q$ which allow for an algebraic solution of the TQ equation (3.18) in the case of nondiagonal boundary conditions.

In the case of particle number conserving diagonal boundary matrices the TQ equation can be solved in terms of Fourier polynomials of fixed degree for the $Q$-functions. Comparing to what is obtained using the algebraic or coordinate Bethe ansatz they are given by [28]–[30]

\[
Q(u) = \prod_{\ell=1}^{M} \sin(u - v_0^{(\ell)}) \sin(u + v_0^{(\ell)} + 2\eta),
\]

(3.21)

for all anisotropies $0 \leq \eta \leq \pi/2$. For small system sizes $N$ we have checked by explicit computation of the functions $Q^{(n)}(u)$ from the recursion relations (3.5) for diagonal
boundary fields that they do in fact converge to the expression (3.21) for \(n \to \infty\) for all anisotropy parameters. The zeros \(v^{(0)}_\ell\) of the \(Q\)-functions are determined by requiring analyticity of the eigenvalues \(\Lambda(u)\) of the transfer matrix from the TQ equation (3.18). This yields the BAE for the diagonal model,

\[
\frac{h^-(v^{(0)}_\ell)}{h^+(v^{(0)}_\ell)} = \frac{Q(v^{(0)}_\ell + 2\eta)}{Q(v^{(0)}_\ell - 2\eta)},
\]

or upon substitution

\[
\left( \frac{\sin(v^{(0)}_\ell + 2\eta)}{\sin v^{(0)}_\ell} \right)^{2N} \frac{\sin(v^{(0)}_\ell + \psi_-) \sin(v^{(0)}_\ell + \psi_+)}{\sin(v^{(0)}_\ell + 2\eta - \psi_+) \sin(v^{(0)}_\ell + 2\eta - \psi_-)}
= \prod_{j \neq \ell}^M \frac{\sin(v^{(0)}_\ell - v^{(0)}_j + 2\eta) \sin(v^{(0)}_\ell + v^{(0)}_j + 4\eta)}{\sin(v^{(0)}_\ell - v^{(0)}_j - 2\eta) \sin(v^{(0)}_\ell + v^{(0)}_j)}.
\]

(3.23)

4. Nondiagonal boundaries

Having reproduced the spectrum of the diagonal model, we now turn our attention to the case where nondiagonal boundary conditions are considered. Based on our findings above we assume that the spectral problem is given by the TQ equation (3.18) for arbitrary values of the anisotropy \(\eta\). It turns out that the incorporation of the nondiagonal contributions can be carried out efficiently by appropriately deforming the \(h\) and \(Q\)-functions of the diagonal model. Thus our starting point would be a deformation of the TQ equations themselves,

\[
\Lambda(u) = H^-(u) \frac{\bar{Q}(u - 2\eta)}{\bar{Q}(u)} - H^+(u) \frac{\bar{Q}(u + 2\eta)}{\bar{Q}(u)},
\]

(4.1)

where the \(\Lambda(u)\) denote the eigenvalues of the full, nondiagonal problem. Regarding the \(H\)-functions first, since the diagonal case should be contained within the construction as a special limit, we propose the following deformations:

\[
H^\pm(u) = h^\pm(u)(1 + \mathcal{G} f^\pm(u)),
\]

(4.2)

where the \(h^\pm(u)\) are given in (3.19), \(\mathcal{G}\) is the combination of the odd Grassmann parameters defined in (2.20) and the \(f^\pm(u)\) are generic functions to be determined. There exist two constraints on the expressions of these unknown functions. First, their contribution in the factorization of the quantum determinant should vanish, yielding

\[
f^+(u - 2\eta) = -f^-(u).
\]

(4.3)

Furthermore, the crossing symmetry of the eigenvalues \(\Lambda(u)\) entailed by (2.16) should be preserved. We therefore assume that the \(\bar{Q}\)-functions enjoy crossing symmetry as well, similarly to the functional (3.18) derived from the truncation identities. This implies that the \(H\)-functions are related through \(H^-(u) = -H^+(u - 2\eta)\). This relation holds automatically for the \(h\)-functions of the diagonal case, whereas it also provides a second constraint on \(f^\pm(u)\),

\[
f^+(u - 2\eta) = f^-(u).
\]

(4.4)
A set of solutions to these functional relations is given by

\[
\begin{align*}
    f^+(u) &= \mathcal{W} \sin(2u + 4\eta), \\
    f^-(u) &= -\mathcal{W} \sin(2u),
\end{align*}
\]  

with the coefficient \( \mathcal{W} \) to be determined from the asymptotic behavior (2.19) of the transfer matrix eigenvalues. It should be stressed that the above choice is not unique, but it was found to be the only one consistent with the various limits and with the constraints arising from the functional relations.

A similar deformation should be considered for the \( \tilde{Q} \)-functions as well, since they are assumed to originate from the higher spin eigenvalues through a limiting procedure. The most general ansatz extending the functions \( Q(u) \) of the diagonal case (3.21) and containing the special combination of Grassmann numbers, \( \mathcal{G} \), reads as

\[
\tilde{Q}(u) = Q(u) + \mathcal{G} b(u),
\]  

with \( b(u) \) being a function to be determined. Substituting the deformations (4.2) and (4.6) into the TQ equation (4.1), the latter becomes

\[
\begin{align*}
    \Lambda(u) &= \Lambda^{\text{diag}}(u) \left( 1 - \mathcal{G} \frac{b(u)}{Q(u)} \right) + \mathcal{G} \left[ h^-(u) \left( \frac{b(u - 2\eta)}{Q(u)} + f^-(u) \frac{Q(u - 2\eta)}{Q(u)} \right) \\
    &\quad - h^+(u) \left( \frac{b(u + 2\eta)}{Q(u)} + f^+(u) \frac{Q(u + 2\eta)}{Q(u)} \right) \right].
\end{align*}
\]  

Additional requirements are needed to determine the function \( b(u) \) in (4.6). Again the choice of this function has to guarantee the analyticity of the additional terms appearing in the functional equation (4.7) for the eigenvalues. In addition, \( b(u) \) should enjoy crossing symmetry, which was assumed in order to derive the constraint (4.4). In this spirit, we propose that the nondiagonal correction to the \( Q \)-functions is given by

\[
b(u) = \prod_{\ell=1}^{M'} \sin(u - v_\ell^{(1)}) \sin(u + v_\ell^{(1)} + 2\eta),
\]  

with \( \{v_\ell^{(1)}\} \neq \{v_\ell^{(0)}\} \) in general. Matching of the asymptotic behavior dictates that the upper limits of the products in equations (4.6) and (4.8) should be equal, \( M' = M \). Furthermore, the asymptotics (2.19) provide the explicit expression for the coefficient \( \mathcal{W} \) as

\[
\mathcal{W} = \frac{1}{\sin[\psi_+ + \psi_- + (N - 2M - 1)2\eta]}.
\]  

Apart from the asymptotics, one should also consider additional limits of the TQ equation in order to check the consistency of the procedure. The limit \( u \to 0 \) gives \( \Lambda(0) = 1 \), which stems from the normalization of the transfer matrix. Setting \( u = 0 \) in the TQ equation, after a quick inspection one is led to the following constraint for \( b(u) \):

\[
b(-2\eta) = b(0),
\]  

which is a special case of a crossing symmetry requirement and is automatically satisfied by the choice (4.8). Finally, it is interesting to consider the semi-classical limit \( \eta \to 0 \). In this
limit the \( b(u) \) functions drop out from the TQ equation and the eigenvalues become

\[
\Lambda(u)_{\eta \to 0} = (h^{-}(u) - h^{+}(u)) + \mathcal{G} f^{-}(u)(h^{-}(u) + h^{+}(u)),
\]

{eq:4.11}

finding perfect agreement with the semi-classical limit obtained from the transfer matrix \((2.18)\), after recalling the expressions for \( h^{\pm}(u) \) \((3.1)\) and \( f^{\pm}(u) \) \((4.5)\) with the coefficient \( \mathcal{W} \) \((4.9)\) for \( \eta \to 0 \).

The parameters \( v^{(1)}_\ell \) in \((4.8)\) are determined by requiring analyticity of the eigenvalues of the full transfer matrix. The purely complex part of the TQ equation \((4.7)\) yields the already derived BAE \((3.23)\), while the one containing Grassmann numbers provides a second set of relations, involving both sets of roots \( v^{(0)}, v^{(1)} \), which reads as

\[
\frac{h^{-}(v^{(0)}_\ell)}{h^{+}(v^{(0)}_\ell)} = \frac{\Lambda^{\text{diag}}(v^{(0)}_\ell) b(v^{(0)}_\ell)}{h^{+}(v^{(0)}_\ell) \left( b(v^{(0)}_\ell) - 2\eta \right) + f^{-}(v^{(0)}_\ell)Q(v^{(0)}_\ell) - 2\eta) \right)}
\]

\[
+ \frac{b(v^{(0)}_\ell) + 2\eta + f^{+}(v^{(0)}_\ell)Q(v^{(0)}_\ell) + 2\eta) \right)}{b(v^{(0)}_\ell) - 2\eta + f^{-}(v^{(0)}_\ell)Q(v^{(0)}_\ell) - 2\eta) \right)}.
\]

{eq:4.12}

Note that the roots \( v^{(0)} \) and \( v^{(1)} \) also enter this set of equations through the functions \( Q(u) \) and \( b(u) \).

In summary, we have two sets of algebraic equations fixing the parameters appearing in the ansatz for \( \tilde{Q}(u) \). These equations are of nested Bethe ansatz type, similar to those appearing in integrable models based on higher rank symmetries. It should be stressed that the expression for the eigenvalues of the super transfer matrix \((4.7)\) and the corresponding BAE \((4.12)\) rely on the conjectural deformations of the \( h \)- and \( Q \)-functions in equations \((4.2)\) and \((4.6)\) respectively. However, we have explicitly verified that our proposed scheme is compatible with the various limits and symmetry requirements, namely the truncation to the diagonal case, the crossing symmetry, the limits \( u \to 0 \) and \( \eta \to 0 \) and the asymptotics of the transfer matrix. Moreover, the deformations of the \( h \)-functions are compatible with the constraints arising from the functional relations, namely equations \((3.12)\), which provides an additional, nontrivial check of our expressions. In order to further enforce the validity of our proposed scheme for the eigenvalues as computed from the TQ equation, we have analytically diagonalized the transfer matrix for a small number of chain lengths. The comparison of the exact eigenvalues with the ones obtained from \((4.7)\) exhibits perfect agreement.

5. The eigenstates of the model

In the previous sections we have obtained the eigenvalues of the transfer matrix from the fusion hierarchy and the resulting TQ equation. Similarly to the case of diagonal boundary matrices the eigenvalues can be associated to sectors labeled by the integer \( M \) of parameters appearing in the solution. This is remarkable since the related \( U(1) \) symmetry is broken when the nondiagonal boundary conditions are applied.

As is common to functional Bethe ansatz approaches our solution of the spectral problem thus far does not provide information regarding the eigenstates of the model. However, exploiting the existence of the odd Grassmann numbers and their nilpotency, it is possible to exactly compute the \( M = 0 \) state of the model for an arbitrary number \( N \)
of chain sites, solely by using the derived expressions of the eigenvalues. To this end we choose $k$-particle states, $k = 0, \ldots, N$,

$$|i_1 i_2 \cdots i_k \rangle \equiv c_{i_1}^\dagger c_{i_2}^\dagger \cdots c_{i_k}^\dagger \Omega, \quad 1 \leq i_1 < i_2 < \cdots < i_k \leq N$$

(5.1)

as the basis of the Hilbert space of the system; $|\Omega\rangle$ is the Fock vacuum of the system (and the $M = 0$ eigenvector of the diagonal problem).

The key observation used for the construction of the unique $M = 0$ eigenvector of the model with nondiagonal boundary conditions is that for generic chain length $N$, only the Fock vacuum and basis states containing one or two particles contribute with non-vanishing amplitudes, all other sectors decouple. This allows us to express the $M = 0$ eigenvector of the nondiagonal model as

$$|\Psi\rangle_{M=0} = |\Omega\rangle + \beta^+ \sum_{i=1}^N b_i^+ |i\rangle + \beta^- \sum_{i=1}^N b_i^- |i\rangle + \beta^+ \beta^- \sum_{i<j}^N B_{ij} |ij\rangle.$$  

(5.2)

The eigenvalue problem for the complete Hamiltonian reads as

$$H |\Psi\rangle = (\lambda_{\text{diag}} + G \lambda_{\text{nondiag}}) |\Psi\rangle.$$  

(5.3)

Splitting the terms with respect to the order of $\beta^\pm$ we obtain

$$\mathcal{O}(\beta): (H_{\text{bulk}} + H_{\text{diag}}) \beta^n \sum_i b_i^n |i\rangle + H_{\text{nondiag}} |\Omega\rangle = \lambda_{\text{diag}} \beta^n \sum_i b_i^n |i\rangle$$

$$\mathcal{O}(\beta^2): (H_{\text{bulk}} + H_{\text{diag}}) \beta^+ \beta^- \sum_{i<j} B_{ij} |ij\rangle + H_{\text{nondiag}} \beta^+ \beta^- \sum_i b_i^n |i\rangle$$

(5.4)

$$= G \lambda_{\text{nondiag}} |\Omega\rangle + \lambda_{\text{diag}} \beta^+ \beta^- \sum_{i<j} B_{ij} |ij\rangle.$$  

Regarding the terms linear in $\beta^\pm$ first, after the relevant computations and splitting the resulting relations with respect to the appropriate excited states, one ends up with the following six relations that determine the coefficients $b_i^\pm$:

$$\beta^+ |1\rangle: - t b_1^+ + b_1^+ [V(N - 2) - \frac{1}{2} \cot \psi_- + \mathcal{N}_+ - \lambda_{\text{diag}}] = 0$$

$$\beta^+ |N\rangle: - t b_{N-1}^+ - \csc \psi_- + b_{N-1}^+ [V(N - 2) + \frac{1}{2} \cot \psi_- - \mathcal{N}_- - \lambda_{\text{diag}}] = 0$$

$$\beta^- |1\rangle: - t b_1^- - \csc \psi_- + b_1^- [V(N - 2) - \frac{1}{2} \cot \psi_- + \mathcal{N}_+ - \lambda_{\text{diag}}] = 0$$

$$\beta^- |N\rangle: - t b_{N-1}^- + b_{N-1}^- [V(N - 2) + \frac{1}{2} \cot \psi_- - \mathcal{N}_- - \lambda_{\text{diag}}] = 0$$

$$\beta^\pm |\ell\rangle: - t (b_{\ell-1}^+ + b_{\ell+1}^+) + b_\ell^\pm [V(N - 3) + \frac{1}{2} \cot \psi_- + \mathcal{N}_+ - \lambda_{\text{diag}}] = 0,$$

(5.5)

where the recursion relations are valid for $2 \leq \ell \leq N - 1$ and can be solved analytically, giving

$$b_\ell^\pm = \frac{1}{2t} \left[ \left( \frac{C_0 - \sqrt{C_0^2 - 4t^2}}{t} \right)^\ell C_1^\pm + \left( \frac{C_0 + \sqrt{C_0^2 - 4t^2}}{t} \right)^\ell C_2^\pm \right],$$

(5.6)

with $C_0 \equiv V(N - 3) + \frac{1}{2} \cot \psi_- + \mathcal{N}_+ - \lambda_{\text{diag}}$ and $C_{1,2}$ constants to be determined. Proceeding to the quadratic terms, the ones proportional to $\beta^+ \alpha^-$ and $\beta^- \alpha^+$ first give the constraints

$$\csc (\psi_-) b_1^+ = \lambda_{\text{nondiag}} = \csc (\psi_-) b_N^+.$$  

(5.7)

These two constraints, combined with the set of relations (5.5) are sufficient to completely determine the constants $C_{1,2}^\pm$ and therefore all coefficients $b_\ell^\pm$. We conclude that the
coefficients $b^\pm_\ell$ are given by

\[
b^+_\ell = -\frac{\sin(\psi_- + (\ell - 1)2\eta)}{\sin((N - 1)2\eta + \psi_- + \psi_+)}
\]

\[
b^-_\ell = -\frac{\sin(\psi_+ + (N - \ell)2\eta)}{\sin((N - 1)2\eta + \psi_- + \psi_+)}.
\]

Concerning the rest of the quadratic terms, after some algebra and splitting the terms with respect to various states, we conclude that the coefficients $B_{k\ell\ell}$ satisfy the following relations:

\[(\Xi^+_q + \mathcal{N}_-)B_{1N} + t(B_{1N-1} + B_{2N}) + b^+_N \csc \psi_- + b^+_1 \csc \psi_+ = 0
\]

\[(\Xi^+_2 + \mathcal{N}_-) B_{1N} + tB_{1N} + b^+_N \csc \psi_+ = 0
\]

\[(\Xi^+_1 + \mathcal{N}_-) B_{1N} + t(B_{1N} + B_{1+1N} + B_{N+1}) + b^+_N \csc \psi_+ = 0, \quad 1 < \ell < N - 1
\]

\[(\Xi^- + \mathcal{N}_+) B_{1\ell} + t(B_{1\ell} + B_{1\ell+1} + B_{2\ell}) + b^-_\ell \csc \psi_- = 0, \quad 2 < \ell < N
\]

\[(\Xi^- - \mathcal{N}_+) B_{\ell+1} + t(B_{\ell+1} + B_{\ell+2}) = 0, \quad 1 < \ell < N - 1
\]

\[(\Xi^- - \mathcal{N}_+) B_{k\ell\ell} + t(B_{k\ell\ell} + B_{k+1\ell} + B_{k\ell+1} + B_{k\ell+1}) = 0, \quad 1 < k < N - 2, \quad \ell > k + 1
\]

where for the sake of readability we have defined

\[\Xi^+q \equiv \lambda_{\text{diag}} \pm \frac{1}{2} \cot \psi_+ - V(N - q).\]  

In principle, having acquired the exact expressions for $b^\pm_\ell$, the above set of relations provides the expressions of $B_{k\ell\ell}$ as well. Since it is hard to solve these relations analytically, one may resort to a numerical analysis for a given number of chain sites. However, solving these equations for small numbers of chain lengths, we were able to observe the emerging pattern which governs the coefficients $B_{k\ell\ell}$. In short, we have found that they are eventually given by the very simple expressions

\[B_{k\ell\ell} = \frac{\sin((N - 1)2\eta + \psi_- + \psi_+)}{\sin((N - 2)2\eta + \psi_- + \psi_+)} (b^+_k b^-_\ell + b^-_k b^+_\ell).\]

We have explicitly confirmed that the expressions (5.10) satisfy all the generic constraints and relations derived above. In conclusion, the $M = 0$ eigenvector of the model is completely determined for an arbitrary number of chain sites.

The decoupling of higher/lower sectors, due to the nilpotency of the Grassmannian parameters, further constrains the expressions of the eigenvectors which correspond to excited states. For generic values of $M$ then, we propose that the corresponding eigenvector will be given by the following schematic expression:

\[
|\Psi\rangle_M = (c_1 + c_2 \alpha^+ \beta^- + c_3 \beta^+ \alpha^-)|M\rangle + c_4 \beta^+|M + 1\rangle + c_5 \beta^-|M + 1\rangle + c_6 \beta^+ \beta^-|M + 2\rangle + c_7 \alpha^+ \alpha^-|M - 1\rangle + c_8 \alpha^-|M - 1\rangle + c_9 \alpha^+ \alpha^-|M - 2\rangle,
\]

where by $|M\rangle$ we denote the states with $M$ particles present, or equivalently the states with $M$ spins down in the spin picture, i.e. $M$ excitations from the ground state. The
number of states with the same $M$ is given by the binomial coefficient

$$\binom{N}{M} = \frac{N!}{M!(N-M)!},$$

so that the states $\vert M \rangle$ in (5.11) are to be understood as collections of states spanning the degeneracy space for a particular $M$. In the same spirit, the coefficients $c_i \in \mathbb{C}$ appearing also in (5.11) are to be interpreted as sets of coefficients of the degenerate states.

6. Discussion

In this work, we have solved the small polaron model with nondiagonal boundary conditions. The eigenvalues of the transfer matrix have been extracted by using the fusion hierarchy of the transfer matrices and also by considering the functional relations for particular values of the anisotropy parameter. Starting from the fusion hierarchy of the transfer matrices together with its truncation at particular values of the anisotropy parameter we have formulated the spectral problem as a functional TQ equation. The latter has been solved by means of appropriate deformations needed to account for the nondiagonal nature of the model. The eigenvalues have been found to depend on two sets of Bethe roots, for which coupled Bethe ansatz equations have been presented.

An interesting aspect of the model’s solution is that, unlike the case of the XXZ model with nondiagonal boundary conditions, no restrictions emerge for the boundary parameters. This extra freedom, as well as the remnants of particle number conservation leading to sectors of the Hilbert space labeled by the integer $M$, appears to be inherited from the supersymmetric nature of the model. Furthermore, supersymmetry heavily restricts the structure of the eigenvectors and has rendered it possible to exactly compute the $M = 0$ eigenstate of the model. A more detailed analysis should provide the complete expressions of all eigenvectors.

Since supersymmetry lifts any possible constraints between the boundary parameters for the small polaron, it is interesting to consider other supersymmetric models with nondiagonal boundaries. Particularly interesting would be an extension of the analysis of the supersymmetric t–J model with open boundaries [35, 36] to this case. In this case nondiagonal terms breaking either the $U(1)$ charge symmetry or the $SU(2)$ spin symmetry of the model can be added. The latter problem has been partially solved by Galleas [37] and leads to problems similar to those encountered in the XXX Heisenberg chain with nondiagonal boundary fields. As to boundary terms breaking the charge symmetry of the model, we expect that they can be dealt with in a similar manner to the small polaron model.

Another route to follow is to consider operator valued representations of the reflection algebras [7, 38, 39] instead of c-number solutions, and attempt to solve the model for boundary conditions breaking the bulk symmetries. The construction of suitable, generalized Jordan–Wigner transformations for the nondiagonal boundary terms would provide valuable information in this spirit.
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Appendix. The Jordan–Wigner transformation

The Jordan–Wigner transformation is a bijective mapping between spin-1/2 operators and fermionic creation/annihilation operators in one-dimensional quantum systems. In the following it will be shown how the small polaron model with periodic and diagonal boundary conditions can be mapped onto an XXZ Heisenberg spin chain by virtue of this very transformation.

Let \( c_j^\dagger \) and \( c_j \) denote the creation and annihilation operators of spinless fermions on the \( j \)th lattice site, subject to the anticommutation relations

\[
\{ c_k^\dagger, c_\ell \} \equiv c_k^\dagger c_\ell + c_\ell c_k^\dagger = \delta_{k\ell}, \quad \{ c_k, c_\ell \} = 0 \quad \text{and} \quad \{ c_k^\dagger, c_\ell^\dagger \} = 0. \tag{A.1}
\]

The Jordan–Wigner transformation expresses these operators in terms of spin-1/2 raising and lowering operators \( S_j^+ \) and \( S_j^- \) at corresponding sites \( j \) by means of

\[
c_j^\dagger = e^{i\phi_j} S_j^- \quad \text{and} \quad c_j = e^{-i\phi_j} S_j^+ \tag{A.2}
\]

where the phase \( \phi_j \) is given by

\[
\phi_j \equiv \pi \sum_{\ell=1}^{j-1} S_\ell^+ S_\ell^- \tag{A.3}
\]

Recall also that \( S_j^\pm = S_j^x \pm i S_j^y \) and \( S_j^x \), \( S_j^y \) and \( S_j^z \) are two-dimensional representations of the \( su(2) \) algebra

\[
[S_\alpha^\beta, S_\gamma^\delta] = i \delta_{\alpha\delta} e^{\alpha\beta\gamma} S_\gamma^\gamma, \quad \alpha, \beta, \gamma \in \{ x, y, z \}. \tag{A.4}
\]

Several useful relations can be deduced directly from these definitions, in particular

\[
n_j \equiv c_j^\dagger c_j = S_j^- S_j^+, \quad c_j^\dagger c_{j+1} = -S_j^- S_{j+1}^+, \\text{ and } \quad \bar{n}_j \equiv c_j c_j^\dagger = S_j^+ S_j^-, \quad c_{j+1}^\dagger c_j = -S_j^+ S_{j+1}^-. \tag{A.5}
\]

According to (2.1) the bulk part of the small polaron model is determined by the Hamiltonian density

\[
H_{j,j+1} = -t \cdot (c_{j+1}^\dagger c_j^\dagger + c_j^\dagger c_{j+1}) + V \cdot (\underbrace{[1 - \bar{n}_{j+1}]}_{n_{j+1}} \cdot \underbrace{[1 - \bar{n}_j]}_{n_j} + \bar{n}_{j+1} \bar{n}_j), \tag{A.6}
\]

which the Jordan–Wigner transformation (A.2) maps to,

\[
H_{j,j+1} = 2t \cdot (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + 2V \cdot S_j^z S_{j+1}^z, \tag{A.7}
\]

which is precisely the Hamiltonian density of the XXZ spin chain.

Along the same lines it is easily shown that the diagonal boundary contributions (2.15) to the open small polaron Hamiltonian, i.e.

\[
H_{\text{diag}} = \mathcal{N}_0 (\bar{n}_1 - n_1) + \mathcal{N}_+ \bar{n}_N - \mathcal{N}_- n_N, \tag{A.8}
\]

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map to

\[ H^{\text{diag}} = 2N_0 S^z_1 + (N_+ + N_-)(S^z_N + \frac{1}{2}). \]  

(A.9)

The fact that \( N_+ \neq N_- \) in the diagonal boundary terms stems from the supersymmetric nature of the model.

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