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Non-diagonal reflection for the non-critical *XXZ* model

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Abstract

The most general physical boundary S-matrix for the open XXZ spin chain in the non-critical regime ($\cosh(\eta) > 1$) is derived starting from the bare Bethe ansatz equations. The boundary S-matrix as expected is expressed in terms of Γ_q-functions. In the isotropic limit the corresponding results for the open XXX chain are also reproduced.

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1. Introduction

The open XXZ model is considered as one of the prototype models in describing a plethora of interesting boundary phenomena, and as such has attracted much attention especially after the derivation of the spectrum in the generic case where non-diagonal boundary magnetic fields are applied [1–5]. Our objective in the present study is to derive from first principles the most general physical boundary S-matrix for the XXZ chain in the non-critical (massive) regime.

Diagonal boundary S-matrices for the open XXZ model in the non-critical regime were extracted in [6] using vertex-operator techniques, while parallel results were obtained in [7] from the Bethe ansatz point of view (see, e.g., [8–10]). Similarly, diagonal reflection matrices were derived in [11, 12] for the critical XXZ model corresponding to the sine-Gordon boundary S-matrix for 'fixed' boundary conditions [13]. After the derivation of the exact spectrum and Bethe equations for the XXZ chain with non-diagonal boundaries the generic boundary S-matrix for the critical XXZ chain was computed in [14, 15] corresponding to the boundary S-matrix of sine-Gordon model [13] for 'free' boundary conditions. A relevant discussion on the generic breather boundary S-matrix within the XXZ framework may also be found in [14]. Note also that analogous results regarding diagonal and non-diagonal solitonic boundary S-matrices were formulated in [16, 17] using the so-called nonlinear integral equation (NLIE) method [18].

To extract the generic boundary S-matrix for the non-critical XXZ model we follow the logic of [14], i.e. we focus on the open chain with a trivial left boundary and a generic non-diagonal right boundary associated with the full K-matrix [13, 19]. As also noted in [14]

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the main advantage of the approach adopted —considering special boundary conditions— is that one eventually deals with a simple set of Bethe ansatz equations similar to those of the *XXZ* chain with two diagonal boundaries. Thus all relevant computations are drastically simplified (see also [14]), and one may follow the logic described in [7, 12, 20, 21] for purely diagonal boundary magnetic fields. Ultimately, the boundary *S*-matrix eigenvalues are extracted directly from the Bethe equations and are expressed in terms of Γ_q-functions ($q = \mathrm{e}^{-\eta}$) [22] as in [6, 7], where only diagonal boundaries are assumed. In the isotropic limit $q \to 1$, the corresponding rational boundary *S*-matrix for the *XXX* open chain is also recovered [23].

2. Bethe ansatz and boundary *S*-matrix

Before we proceed with the Bethe ansatz analysis it will be useful for our purposes here to give the explicit expressions of the right and left boundary *K*-matrices that give rise to the open Hamiltonian under consideration:

$$\mathcal{H} = -\frac{1}{4}\sum_{i=1}^{N-1}\left(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \cosh(\eta)\sigma_i^z\sigma_{i+1}^z\right) - \frac{N}{4}\cosh(\eta) + \frac{\sinh(\eta)}{4}\sigma_N^z + \frac{\sinh(\eta)\cosh(\eta\xi)}{4\sinh(\eta\xi)}\sigma_1^z - \frac{\kappa\sinh(\eta)}{2\sinh(\eta\xi)}\left(\cosh(\eta\theta)\sigma_1^x + \mathrm{i}\sinh(\eta\theta)\sigma_1^y\right) \tag{2.1}$$

where in the non-critical regime we are focusing here $\cosh(\eta) > 1$, also $\sigma^{x,y,z}$ are the 2×2 Pauli matrices, and the boundary parameters ξ, κ, θ are the free parameters of the generic *K*-matrix [13, 19], which will be introduced subsequently.

To obtain such a Hamiltonian we consider the open chain constructed using Sklyanin's formalism [24], with left boundary $K^+ \propto \mathrm{I}$ and right boundary associated with the general solution of the reflection equation [25] given in [13, 19], i.e.,

$$K^-(\lambda) = \begin{pmatrix} \sin[\eta(-\lambda + \mathrm{i}\xi)]\,\mathrm{e}^{\mathrm{i}\eta\lambda} & \kappa\,\mathrm{e}^{\eta\theta}\sin(2\eta\lambda) \\ \kappa\,\mathrm{e}^{-\eta\theta}\sin(2\eta\lambda) & \sin[\eta(\lambda + \mathrm{i}\xi)]\,\mathrm{e}^{-\mathrm{i}\eta\lambda} \end{pmatrix}. \tag{2.2}$$

The latter *K*-matrix has two eigenvalues given as follows:

$$\begin{aligned} \varepsilon_1(\lambda) &= 2\kappa\sin[\eta(\lambda + \mathrm{i}p^+)]\sin[\eta(\lambda + \mathrm{i}p^-)] \\ \varepsilon_2(\lambda) &= 2\kappa\sin[\eta(\lambda - \mathrm{i}p^+)]\sin[\eta(\lambda - \mathrm{i}p^-)] \end{aligned} \tag{2.3}$$

where the parameters $p^\pm$ are defined as:

$$\frac{\mathrm{e}^{\pm\eta\xi}}{2\kappa} = \mathrm{i}\cosh[\eta(p^+ \pm p^-)]. \tag{2.4}$$

Note that we assume here the parametrization used in [13] in the sine-Gordon context, (see also [14] and the references therein). Such a parametrization is also quite practical within the Temberley–Lieb algebra framework [26]. The parameter θ appearing in (2.2) may be removed by means of a simple gauge transformation, that leaves the *XXZ* *R*-matrix invariant, and henceforth we consider it for simplicity to be zero (see also [13, 14]). The *K*-matrix (2.2) may be easily diagonalized by virtue of a constant (λ-independent) gauge transformation:

$$\mathrm{diag}(\varepsilon_1(\lambda), \varepsilon_2(\lambda)) = \mathcal{M}^{-1}(p^+, p^-)K(\lambda)\mathcal{M}(p^+, p^-) \tag{2.5}$$

where $\mathcal{M}$ is defined as

$$\mathcal{M}(p^+, p^-) = \begin{pmatrix} 1 & 1 \\ \mathrm{i}\,\mathrm{e}^{\eta(p^+ + p^-)} & \mathrm{i}\,\mathrm{e}^{-\eta(p^+ + p^-)} \end{pmatrix}. \tag{2.6}$$

Note that the above transformation modifies dramatically the *XXZ R*-matrix, so it is not possible to simply implement a global gauge transformation changing the basis in order to diagonalize the open transfer matrix as in, e.g., [27]. It is also worth pointing out the similarity between the matrix $\mathcal{M}(p^+, p^-)$ and the local gauge transformation employed for the diagonalization of the open *XXZ* transfer matrix with non-diagonal boundaries [1, 28, 29].

We recall now the exact Bethe ansatz equations for the open *XXZ* chain in the case of a right non-diagonal boundary and a left trivial diagonal. The Bethe equations in this case reduce to the following simple form (see also [14]):

$$\frac{\sin\left[\eta\left(\lambda_i - \frac{\mathrm{i}}{2}(2p^+ + 1)\right)\right]}{\sin\left[\eta\left(\lambda_i + \frac{\mathrm{i}}{2}(2p^+ + 1)\right)\right]} \frac{\sin\left[\eta\left(\lambda_i - \frac{\mathrm{i}}{2}(2p^- + 1)\right)\right]}{\sin\left[\eta\left(\lambda_i + \frac{\mathrm{i}}{2}(2p^- + 1)\right)\right]} \frac{\cos\left[\eta\left(\lambda_i + \frac{\mathrm{i}}{2}\right)\right]}{\cos\left[\eta\left(\lambda_i - \frac{\mathrm{i}}{2}\right)\right]} \left(\frac{\sin\left[\eta\left(\lambda_i + \frac{\mathrm{i}}{2}\right)\right]}{\sin\left[\eta\left(\lambda_i - \frac{\mathrm{i}}{2}\right)\right]}\right)^{2N+1}$$
$$= -\prod_{j=1}^{M} \frac{\sin[\eta(\lambda_i - \lambda_j + \mathrm{i})]}{\sin[\eta(\lambda_i - \lambda_j - \mathrm{i})]} \frac{\sin[\eta(\lambda_i + \lambda_j + \mathrm{i})]}{\sin[\eta(\lambda_i + \lambda_j - \mathrm{i})]}. \tag{2.7}$$

We consider here, without loss of generality $\eta > 0$, $p^{\pm} > \frac{1}{2}$ and $\mathrm{Re}\,(\lambda_\alpha) \in \left[0, \frac{\pi}{2\eta}\right]\lambda_\alpha \neq 0, \frac{\pi}{2\eta}$ (see, e.g., [20] for details on this restriction). For relevant results on various representations of $U_q(sl_2)$ see [28–30].

As pointed out in [14] the integer M is associated with a non-local conserved quantity $\mathcal{S}$, which has the same spectrum as S^z (for more details we refer the interested reader to [14, 28] and references therein), i.e.,

$$M = \frac{N}{2} - \mathcal{S}_\varepsilon, \tag{2.8}$$

the subscript ε stands for the eigenvalue.

Our objective now is to explicitly derive the physical boundary *S*-matrix, and in particular the relevant overall physical factor, which provides in general significant information on the existence of boundary bound states. We define the boundary *S*-matrices $k^{\pm}$ by the quantization condition [10, 20]

$$(\mathrm{e}^{\mathrm{i}2p(\tilde{\lambda})N}\, k^+k^- - 1)|\tilde{\lambda}\rangle = 0. \tag{2.9}$$

Here $\tilde{\lambda}$ is the rapidity of the 'hole' –particle-like excitation and $p(\tilde{\lambda})$ is the momentum of the hole.

The density of a state is obtained in a standard way from the Bethe ansatz equations after taking the log and the derivative [7, 9, 10, 20, 21]. More precisely, the Fourier transform of the density for the one-hole state turns out to be

$$\hat{\sigma}_s(\omega) = 2\hat{\epsilon}(\omega) + \frac{1}{N}\frac{\hat{a}_2(\omega)}{1+\hat{a}_2(\omega)}(\mathrm{e}^{\mathrm{i}\omega\tilde{\lambda}} + \mathrm{e}^{-\mathrm{i}\omega\tilde{\lambda}})$$
$$+ \frac{1}{N}\frac{1}{1+\hat{a}_2(\omega)}[\hat{a}_1(\omega) + \hat{a}_2(\omega) + \hat{b}_1(\omega) - \hat{a}_{2p^-+1}(\omega) - \hat{a}_{2p^++1}(\omega)], \tag{2.10}$$

where we define the following Fourier transforms

$$\hat{a}_n(\omega) = \mathrm{e}^{-\eta n|\omega|}, \qquad \hat{b}_n(\omega) = (-)^{\omega}\hat{a}_n(\omega), \qquad \hat{\epsilon}(\omega) = \frac{\hat{a}_1(\omega)}{1+\hat{a}_2(\omega)} = \frac{1}{2\cosh\left(\frac{\omega}{2}\right)} \tag{2.11}$$

where $\epsilon(\tilde{\lambda})$ corresponds also to the energy of the particle-like excitation. The similarity of the latter formula (2.10) with the one obtained in the case of two diagonal boundaries [7, 20] is indeed noticeable. This is a crucial point enabling a simplified derivation of the boundary *S*-matrix. In our case both terms depending on $p^{\pm}$ are assigned to the right boundary, otherwise one follows the logic of the fully diagonal case (see e.g. [7, 20]).

The boundary matrix k^-, of the generic form (2.2) has two eigenvalues $k_{1,2}$ whereas the left boundary matrix is trivial $k^+(\tilde{\lambda}) = k_0(\tilde{\lambda})\mathrm{I}$. From the density (2.10), the quantization condition (2.9) and recalling that $\epsilon(\lambda) = \frac{1}{2\pi}\frac{\mathrm{d}p(\lambda)}{\mathrm{d}\lambda}$ we can explicitly derive the quantities $k_0, k_{1,2}$ (see, e.g. [7, 20, 21] for more details). Actually, the eigenvalues $k_1(\tilde{\lambda}, p^\pm)$ and $k_2(\tilde{\lambda}, p^\pm)$ may be seen as the boundary scattering amplitudes for the one particle-like excitation with $\mathcal{S} = +\frac{1}{2}$ and $\mathcal{S} = -\frac{1}{2}$, respectively (see also [14] for more details).

We first compute the eigenvalue k_1, which is expressed in terms of the $\Gamma_q(x)$-function, —the q-analogue of the Euler gamma function— ($q = \mathrm{e}^{-\eta}$) defined [22] as

$$\Gamma_q(x) = (1-q)^{1-x}\prod_{j=0}^{\infty}\left[\frac{(1-q^{1+j})}{(1-q^{x+j})}\right], \qquad 0 < q < 1. \tag{2.12}$$

Using also the q-analogue of the duplication formula [22]

$$\Gamma_q(2x)\Gamma_{q^2}\left(\tfrac{1}{2}\right) = (1+q)^{2x-1}\Gamma_{q^2}(x)\Gamma_{q^2}\left(x+\tfrac{1}{2}\right), \tag{2.13}$$

we obtain the following result for the first eigenvalue $k_1(\tilde{\lambda}, p^+, p^-)$ (up to a constant phase factor):

$$\begin{aligned} k_1(\tilde{\lambda}, p^+, p^-) &= 2\kappa \sin\left[\eta\left(\tilde{\lambda} + \frac{\mathrm{i}}{2}(2p^+ - 1)\right)\right]\sin\left[\eta\left(\tilde{\lambda} + \frac{\mathrm{i}}{2}(2p^- - 1)\right)\right] \\ &\quad \times k_0(\tilde{\lambda})k_1(\tilde{\lambda}, p^+)k_1(\tilde{\lambda}, p^-) \end{aligned} \tag{2.14}$$

where we define:

$$k_0(\tilde{\lambda}) = q^{-4\mathrm{i}\tilde{\lambda}}\frac{\Gamma_{q^8}\left(\frac{-\mathrm{i}\tilde{\lambda}}{2} + \frac{1}{4}\right)}{\Gamma_{q^8}\left(\frac{\mathrm{i}\tilde{\lambda}}{2} + \frac{1}{4}\right)}\frac{\Gamma_{q^8}\left(\frac{\mathrm{i}\tilde{\lambda}}{2} + 1\right)}{\Gamma_{q^8}\left(\frac{-\mathrm{i}\tilde{\lambda}}{2} + 1\right)} \tag{2.15}$$

$$k_1(\tilde{\lambda}, x) = \frac{(2\kappa)^{-\frac{1}{2}}}{\sin\left[\eta\left(\tilde{\lambda} - \frac{\mathrm{i}}{2}(2x-1)\right)\right]}\frac{\Gamma_{q^4}\left(\frac{-\mathrm{i}\tilde{\lambda}}{2} + \frac{1}{4}(2x-1)\right)}{\Gamma_{q^4}\left(\frac{\mathrm{i}\tilde{\lambda}}{2} + \frac{1}{4}(2x-1)\right)}\frac{\Gamma_{q^4}\left(\frac{\mathrm{i}\tilde{\lambda}}{2} + \frac{1}{4}(2x+1)\right)}{\Gamma_{q^4}\left(\frac{-\mathrm{i}\tilde{\lambda}}{2} + \frac{1}{4}(2x+1)\right)}. \tag{2.16}$$

We turn now to the computation of the second eigenvalue $k_2(\tilde{\lambda}, p^\pm)$, corresponding to a one-hole state with $\mathcal{S} = -\frac{1}{2}$. We implement the 'duality' transformation [14, 24], which modifies the boundary parameters $p^\pm \to -p^\pm$ in the Bethe ansatz equations (2.7). This transformation is the equivalent of deriving the Bethe ansatz equations starting from the second reference state (the analogue of the 'spin down' state) [30, 31]. Then we conclude for the second eigenvalue:

$$\frac{k_1(\tilde{\lambda}, p^+, p^-)}{k_2(\tilde{\lambda}, p^+, p^-)} = \frac{\sin\left[\eta\left(\tilde{\lambda} + \frac{\mathrm{i}}{2}(2p^+ - 1)\right)\right]\sin\left[\eta\left(\tilde{\lambda} + \frac{\mathrm{i}}{2}(2p^- - 1)\right)\right]}{\sin\left[\eta\left(\tilde{\lambda} - \frac{\mathrm{i}}{2}(2p^+ - 1)\right)\right]\sin\left[\eta\left(\tilde{\lambda} - \frac{\mathrm{i}}{2}(2p^- - 1)\right)\right]} \tag{2.17}$$

An alternative way to extract the second eigenvalue is instead of the 'kink' state with $\mathcal{S} = -\frac{1}{2}$, —after implementing the duality transformation— to consider the anti-kink state consisting of a hole and a two-string state. Such configurations have been utilized in deriving the kink–antikink scattering amplitudes in the bulk *XXZ* model (see, e.g., [7]) as well as in open *XXZ* chain with the most general boundary conditions [15], where the 'duality' $p^\pm \to -p^\pm$ cannot be implemented for the derivation of the second eigenvalue of the boundary *S*-matrix. Note that the term depending on the boundary parameters (2.16) is 'double' compared to the diagonal case studied in [6, 7]. Analogous phenomenon occurs in the open critical *XXZ* chain [14, 15] and the sine-Gordon model [13]. It is straightforward to see that in the diagonal limit we recover the results of [6, 7]. Also, in the isotropic limit $q \to 1, \Gamma_q(x) \to \Gamma(x)$ and the trigonometric functions turn to rational, hence the generic rational reflection matrix for the open *XXX* spin chain is easily recovered (see also [23]).

It is finally convenient to rewrite the two eigenvalues in terms of 'renormalized' boundary parameters $\tilde{p}^{\pm}$ defined as

$$\tilde{p}^{\pm} = p^{\pm} - \frac{1}{2}\mathrm{mod}\left(\frac{\mathrm{i}\pi}{\eta}\right) \tag{2.18}$$

then the similarity between (2.17) and the ratio of the 'bare' eigenvalues (2.3) becomes apparent. We have actually derived the physical boundary S-matrix up to a gauge transformation; indeed the S-matrix of the generic form (2.2) may be reproduced by:

$$k(\lambda, \tilde{p}^{+}, \tilde{p}^{-}) = \mathcal{M}(\tilde{p}^{+}, \tilde{p}^{-})\mathrm{diag}(k_1(\lambda), k_2(\lambda))\mathcal{M}^{-1}(\tilde{p}^{+}, \tilde{p}^{-}), \tag{2.19}$$

$\mathcal{M}$ is defined in (2.5). This concludes our derivation of the general boundary S-matrix for the open *XXZ* chain in the non-critical regime.

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