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Rajan Murgan
University of Miami, rmurgan@physics.miami.edu

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Rajan Murgan

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Rajan Murgan

Approved:

Dr. Rafael Nepomechie
Professor of Physics

Dr. Terri A. Scandura
Dean of the Graduate School

Dr. Orlando Alvarez
Professor of Physics

Dr. James Nearing
Professor of Physics

Dr. Changrim Ahn
Professor of Physics
Ewha Womans University

RAJAN MURGAN (Ph.D., Physics)

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The open spin-$\frac{1}{2}$ XXZ quantum spin chain with general integrable boundary terms is a fundamental integrable model. Finding a Bethe Ansatz solution for this model has been a subject of intensive research for many years. Such solutions for other simpler spin chain models have been shown to be essential for calculating various physical quantities, e.g., spectrum, scattering amplitudes, finite size corrections, anomalous dimensions of certain field operators in gauge field theories, etc.

The first part of this dissertation focuses on Bethe Ansatz solutions for open spin chains with nondiagonal boundary terms. We present such solutions for some special cases where the Hamiltonians contain two free boundary parameters. The functional relation approach is utilized to solve the models at roots of unity, i.e., for bulk anisotropy values $\eta = \frac{i\pi}{p+1}$ where p is a positive integer. This approach is then used to solve open spin chain with the most general integrable boundary terms with six boundary parameters, also at roots of unity, with no constraint among the boundary parameters.

The second part of the dissertation is entirely on applications of the newly obtained Bethe Ansatz solutions. We first analyze the ground state and compute

the boundary energy (order 1 correction) for all the cases mentioned above. We extend the analysis to study certain excited states for the two-parameter case. We investigate low-lying excited states with one hole and compute the corresponding Casimir energy (order $\frac{1}{N}$ correction) and conformal dimensions for these states. These results are later generalized to many-hole states. Finally, we compute the boundary S-matrix for one-hole excitations and show that the scattering amplitudes found correspond to the well known results of Ghoshal and Zamolodchikov for the boundary sine-Gordon model provided certain identifications between the lattice parameters (from the spin chain Hamiltonian) and infrared (IR) parameters (from the boundary sine-Gordon S-matrix) are made.

To my parents

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Chapter 1: Introduction

Exact solutions to some fundamental physical systems such as the hydrogen atom and the harmonic oscillator have played crucial roles in the development of physics. Sytems that can be solved exactly are said to be "integrable." Such exact solutions allow many of the physical properties of these systems such as the spectrum, scattering amplitudes, correlation functions, etc., to be determined exactly without resorting to any sort of approximation methods. Historically, Yang [1] in his solution of the problem of particles in one dimension with repulsive delta function interaction and Baxter [2] in his solution of the eight vertex statistical model independently showed that these integrable models satisfy a special non-linear equation, known as the Yang-Baxter equation (YBE). This equation is a crucial condition of integrability. The YBE also arises as the condition of factorizability of the multiparticle S-matrix of $1 + 1$ dimensional integrable quantum field theory models, such as the sine-Gordon model [3]. For systems with boundary, Zamolodchikov and Cherednik [4, 5] introduced the reflection equation, also known as the boundary Yang-Baxter equation (BYBE), that ensures boundary integrability. Ghoshal and Zamolodchikov [6] demonstrated such boundary integrability in certain $1 + 1$ dimensional boundary quantum field theories through their formulation of boundary scattering matrices that obey BYBE.

A quantum spin chain is a fundamental prototype of integrable models. Such chains come with two topologies, "closed" and "open." Originally, Heisenberg [7] introduced the isotropic closed spin-$\frac{1}{2}$ XXX quantum spin chain in 1928. A few years later, Bethe proposed an ansatz, called Bethe's hypothesis, to solve the model [8]. Hulthen studied the antiferromagnetic ground state of this model [9] using Bethe's hypothesis. This method, now known as the coordinate Bethe Ansatz, was later used by others to obtain further important results on closed spin-$\frac{1}{2}$ XXX and XXZ (anisotropic) spin chains [10]–[13]. Gaudin and Alcaraz et al. utilized the method to solve the open spin-$\frac{1}{2}$ XXZ quantum spin chain with diagonal boundary terms [14, 15] It also served as an important tool to study other models, e.g. delta-function interaction problem [16].

Bethe Ansatz has since been a powerful method to solve integrable models. Over the years, it has been subjected to numerous investigations and applied to solve many quantum systems. In the late 1970's, an alternative method with common mathematical background to coordinate space Bethe Ansatz was devised. This method, which relies on diagonalization of transfer matrices, is known as the Quantum Inverse Scattering Method (QISM) or the algebraic Bethe ansatz (ABA) [17]–[22]. It requires a reference state from which the desired Bethe states can be constructed. ABA has been used to solve many simpler quantum spin chain models, e.g., open spin-$\frac{1}{2}$ XXZ quantum spin chain with diagonal boundary terms [23]. However, obtaining such a reference state for more general quantum spin chains has proven to be a formidable task and still is an open problem. Recently, an ABA solution for the corresponding open spin chain with nondiagonal boundary terms with *constrained* boundary parameters was proposed [24], where a proper "reference" state for this model was found. This Bethe Ansatz solution was also derived using certain functional relations [27, 28] and the Q-operator [29], which do not require the construction of reference states.

We note that Bethe Ansatz is only one of the possible routes towards integrability. Recently, Baseilhac and Koizumi [30] and Galleas [31] proposed solutions for the generic case of the open spin-$\frac{1}{2}$ XXZ quantum spin chain using q-Onsager algebra and nonlinear algebraic relations, respectively. However, computations of thermodynamic properties such as finite size corrections and S-matrices using these methods are still unclear at the present. In this dissertation, we restrict our investigation of integrable quantum spin chains using strictly Bethe-Ansatz-type solutions derived from functional relations. In the following sections of this chapter, some of the above-mentioned results will be briefly reviewed.

1.1 Conditions of integrability

For quantum integrable models, YBE and BYBE ensure bulk and boundary (for models involving boundaries) integrability, respectively. These are nonlinear equations involving $R(u)$ and $K(u)$ matrices, which are the solutions of these equations [1]. The matrix $R(u)$ is defined as an operator acting on the tensor product space $V \otimes V$, where V generally is a $\mathcal{N}$-dimensional complex vector space $\mathcal{C}_{\mathcal{N}}$. Similarly, the matrix $K(u)$ is defined as an operator acting on V. We review them separately below.

1.1.1 Yang-Baxter equation

We first define the permutation matrix, $\mathcal{P} x \otimes y = y \otimes x$ for all vectors x and y. The YBE can be written as

$$R_{12}(u-v) R_{13}(u) R_{23}(v) = R_{23}(v) R_{13}(u) R_{12}(u-v) \tag{1.1}$$

where R_{ij} are operators on $V \otimes V \otimes V$, with $R_{12} = R \otimes 1\,, R_{23} = 1 \otimes R$ and $R_{13} = \mathcal{P}_{23} R_{12} \mathcal{P}_{23}$, where $\mathcal{P}_{23} = 1 \otimes \mathcal{P}$ is the permutation matrix acting nontrivially on the second and third spaces and trivially on the first. Evidently, R_{12} acts nontrivially on the first and second spaces and trivially on the third. Similarly, R_{13} acts nontrivially on the first and third spaces and trivially on the second, etc.

[1]Studies on YBE and BYBE and their solutions have significantly advanced the subject of quantum groups, where these solutions arise from the representations of the quantum groups.

The independent variable u (or v) is called the "spectral parameter." One can interpret (1.1) as factorized scattering of three particles in bulk [3]. As we shall see, the trigonometric solution with $V = \mathcal{C}_2$ of the YBE is of particular interest to us since it yields the R matrix of the spin-$\frac{1}{2}$ XXZ quantum spin chain given below,

$$R(u) = \begin{pmatrix} a & 0 & 0 & 0 \\ 0 & b & c & 0 \\ 0 & c & b & 0 \\ 0 & 0 & 0 & a \end{pmatrix}, \tag{1.2}$$

where

$$a = \sinh(u + \eta)\,, \quad b = \sinh u\,, \quad c = \sinh \eta \tag{1.3}$$

and η is the bulk anisotropy parameter.

1.1.2 Boundary Yang-Baxter equation

The BYBE can be written as [4, 5]

$$R_{12}(u-v)K_1(u)R_{21}(u+v)K_2(v) = K_2(v)R_{12}(u+v)K_1(u)R_{21}(u-v) \tag{1.4}$$

where R_{ij} is defined as before. The matrix $K(u)$ acts on space V, with $K_1 = K \otimes 1\,, K_2 = 1 \otimes K$. As usual, u and v are spectral parameters. Analogous to the YBE (1.1), the BYBE (1.4) can be seen as scattering of particles from a boundary. As for the YBE, various solutions of the BYBE have been found. The most general matrix $K(u)$ of the open spin-$\frac{1}{2}$ XXZ quantum spin chain was found by de Vega and González-Ruiz [32] and independently by Goshal and Zamolodchikov [6] by solving (1.4) directly using the R matrix (1.2).

1.2 Spin-$\frac{1}{2}$ XXZ quantum spin chains

Construction of spin chains requires two crucial "building blocks", namely the R and K matrices introduced above. In the following sections, we review the construction of both the closed and open spin-$\frac{1}{2}$ XXZ quantum spin chains from these matrices.

1.2.1 Closed spin chain

The closed spin-$\frac{1}{2}$ XXZ chain is constructed from only the R matrix (1.2). The transfer matrix can be expressed as

$$t(u) = \mathrm{tr}_0 \, T_0(u) \tag{1.5}$$

where $T_0(u)$ is the monodromy matrix defined as a product of R matrices,

$$T_0(u) = R_{0N}(u) \cdots R_{01}(u) \tag{1.6}$$

where $R_{0n}(u)$ is an operator on

$$\overset{\overset{0}{\downarrow}}{V} \otimes \overset{\overset{1}{\downarrow}}{V} \cdots \otimes \overset{\overset{n}{\downarrow}}{V} \otimes \cdots \otimes \overset{\overset{N}{\downarrow}}{V} \tag{1.7}$$

where "0" is the "auxiliary space" over which the trace tr_0 is taken, and n takes the values of $1\,, 2\,\ldots, N$ representing the "quantum spaces." The monodromy matrix obeys the fundamental relation

$$R_{00'}(u-v) T_0(u) T_{0'}(v) = T_{0'}(v) T_0(u) R_{00'}(u-v) \tag{1.8}$$

which can be proven using (1.1) and the fact that R_{0n} commutes with $R_{0'n'}$ for $n \neq n'$. The transfer matrix has the following important commutativity property

$$[t(u), t(v)] = 0 \tag{1.9}$$

The Hamiltonian can be constructed from the logarithmic derivative of the transfer matrix,

$$\mathcal{H} \;\; = \;\; \sinh\eta \frac{d}{du} \log t(u)|_{u=0} - \frac{N}{2} \cosh\eta \hat{\mathbf{I}}$$

$$
\begin{aligned}
&= \sum_{n=1}^{N-1} H_{n,n+1} + H_{N,1} \,, \\
H_{ij} &= \sinh\eta \mathcal{P}_{ij} R'_{ij}(0) - \frac{1}{2}\cosh\eta \hat{\mathbf{I}} \\
&= \frac{1}{2}\left(\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \cosh\eta\ \sigma_n^z \sigma_{n+1}^z\right) \qquad (1.10)
\end{aligned}
$$

where σ^x , σ^y , σ^z are the standard Pauli matrices, η is the bulk anisotropy parameter, and the prime indicates differentiation with respect to the spectral parameter. One then can readily conclude that $[\mathcal{H}, t(u)] = 0$.

1.2.2 Open spin chain

The transfer matrix $t(u)$ of the open spin chain is given by [23]

$$
t(u) = \mathrm{tr}_0\, K_0^+(u) T_0(u) K_0^-(u) \hat{T}_0(u), \qquad (1.11)
$$

where $T_0(u)$ and $\hat{T}_0(u)$ are the monodromy matrices,

$$
T_0(u) = R_{0N}(u) \cdots R_{01}(u) \,, \quad \hat{T}_0(u) = R_{01}(u) \cdots R_{0N}(u), \qquad (1.12)
$$

and tr_0 again denotes trace over the "auxiliary space" 0. $K^+(u)$ and $K_-(u)$ are the K matrices corresponding to the left and right boundaries of the open spin chain, respectively. One can relate the transfer matrix to the open spin chain Hamiltonian $\mathcal{H}$ using (see [23])

$$
t'(0) = 2\mathcal{H}\, \mathrm{tr}\, K^+(0) + \mathrm{tr}\, K^+(0)' \qquad (1.13)
$$

More discussions on these subjects are found in subsequent chapters where solutions of open XXZ spin chains and applications of these solutions are presented.

1.3 Algebraic Bethe Ansatz

In this section, we review the ABA approach, applied to the case of the closed spin-$\frac{1}{2}$ XXZ spin chain. A crucial element to this approach is the R matrix (1.2) discussed above. Detailed information on this approach can be found in [22]. The monodromy matrix $T_0(u)$ is a 2×2 matrix in the auxiliary space,

$$T_0(u) = \begin{pmatrix} A(u) & B(u) \\ C(u) & D(u) \end{pmatrix}, \tag{1.14}$$

where the elements of this matrix are operators acting on the quantum space $V^{\otimes N}$. These operators obey the following set of algebraic relations encoded in (1.8),

$$[B(u), B(v)] = 0$$

$$\begin{aligned} A(u)B(v) &= \frac{a(v-u)}{b(v-u)} B(v)A(u) - \frac{c(v-u)}{b(v-u)} B(u)A(v)\,, \\ D(u)B(v) &= \frac{a(u-v)}{b(u-v)} B(v)D(u) - \frac{c(u-v)}{b(u-v)} B(u)D(v)\,, \end{aligned} \tag{1.15}$$

where a, b and c are given by (1.3).

The following reference state ω_+ (ferromagnetic state with all spins up) is an eigenstate of $A(u)$ and $D(u)$

$$\omega_+ = \underbrace{\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}}_{N} \tag{1.16}$$

namely,

$$A(u)\omega_+ = \sinh^N(u+\eta)\omega_+\,, \quad D(u)\omega_+ = \sinh^N(u)\omega_+ \tag{1.17}$$

Further, it is annihilated by $C(u)$, $C(u)\omega_+ = 0$. $B(u)$ can be used as a creation operator to form so-called Bethe states,

$$B(u_1)\cdots B(u_M)\omega_+ = |u_1, \ldots, u_M\rangle. \tag{1.18}$$

From (1.5), (1.14)-(1.18), it can be shown that the Bethe state $|u_1, \ldots, u_M\rangle$ is an eigenstate of the transfer matrix $t(u) = A(u) + D(u)$,

$$t(u)|u_1, \ldots, u_M\rangle = \Lambda(u; u_1, \ldots, u_M)|u_1, \ldots, u_M\rangle \tag{1.19}$$

with the eigenvalue

$$\Lambda(u;u_1,\ldots,u_M)=\sinh^N(u+\eta)\frac{Q(u-\eta)}{Q(u)}+\sinh^N(u)\frac{Q(u+\eta)}{Q(u)} \tag{1.20}$$

provided the zeros u_α of the function

$$Q(u)=\prod_{\alpha=1}^{M}\sinh(u-u_\alpha) \tag{1.21}$$

satisfy the following Bethe Ansatz equations,

$$\Big(\frac{\sinh(u_\beta+\eta)}{\sinh(u_\beta)}\Big)^N=-\prod_{\alpha=1}^{M}\frac{\sinh(u_\beta-u_\alpha+\eta)}{\sinh(u_\beta-u_\alpha-\eta)}\qquad \beta=1,\ldots,M,$$
$$0\le M\le\frac{N}{2} \tag{1.22}$$

which also naturally arise from the analyticity of the eigenvalue $\Lambda(u;u_1,\ldots,u_M)$. Quantities of interest such as the energy can now be calculated from the solution of (1.22) using

$$E=\sinh^2\eta\sum_{\alpha=1}^{M}\frac{1}{\sinh(u_\alpha+\eta)\sinh(u_\alpha)}+\frac{N}{2}\cosh\eta \tag{1.23}$$

which can be derived from (1.10) and (1.20). Equations (1.20) and (1.22) are the desired solution of this model that one could use to compute further various physical quantities of the quantum spin chain e.g., bulk scattering amplitudes of spinons. In the following chapters, we shall derive such Bethe Ansatz type equations for more general open quantum XXZ spin chains and utilize these solutions to determine various important physical quantities. Completeness of these solutions can be numerically checked for small number of sites using a method which we describe below.

1.4 McCoy's method

In this section, we describe a method pioneered by Barry McCoy and his collaborators [33, 34], known as 'McCoy's method', to check completeness of Bethe

Ansatz type solutions. It is based on the transfer matrix of the model. One works with newly defined spectral parameters, $x \equiv e^u$ and bulk anisotropy parameter, $q \equiv e^\eta$. McCoy's method consists of four main steps (cf.[28]):

(a) We fix an arbitrary (generic) value x_0 of the spectral parameter, for which we compute the eigenvectors $|\Lambda\rangle$ of the transfer matrix $t(x_0)$. These eigenvectors are independent of the spectral parameter (due to the commutativity property of the transfer matrix (1.9)).

(b) Next, we determine the eigenvalues $\Lambda(x)$ as Laurent polynomials in x by acting with $t(x)$ on the eigenvectors found in (a).

(c) We further set $Q(x) = \sum_{k=-M}^{M} a_k x^k$ (from (1.21)), and determine the coefficients a_k from the relation (1.20), i.e., $\Lambda(x)Q(x) = h(xq)Q(\frac{x}{q}) + h(x)Q(xq)$, where $h(x) = (\frac{x-x^{-1}}{2})^N$.

(d) Finally, we factor the polynomials $Q(x)$, the zeros of which are the Bethe roots one is looking for.

We tabulate results (energy and Bethe roots) for the ground state of the closed spin-$\frac{1}{2}$ XXZ quantum spin chain with even N, obtained using this method in Table 1.1. We also demonstrate the completeness of the solution (1.22) numerically for $N = 4$ in Table 1.2. The number of Bethe roots M is not fixed and is related to the spin S_z,

$$S_z = \pm(\frac{N}{2} - M) \tag{1.24}$$

The "±" can be attributed to the charge conjugation symmetry of the model. This symmetry also implies a two-fold degeneracy of states with nonzero S_z, e.g., in Table 1.2., states with $E = -2.0$ and 2.0 are two-fold degenerate, with spin $S_z = \pm 1$. Another example is the reference state with all spin up (or down) with $M = 0$, namely $S_z = +2$ (or $S_z = -2$) which also gives the two-fold degeneracy. The nondegenerate states, e.g., $E = -3.62258$ and 2.20837 have $S_z = 0$, giving

$M = 2$. Finally, note that there also exist states with much higher degeneracy, e.g., $E = 0$. For these states, in addition to energy and spin, other quantities like the momentum should be taken into consideration to distinguish them.

N	M	ground state energy, E	shifted Bethe roots $\tilde{u_\alpha} = u_\alpha + \frac{\eta}{2}$
2	1	-2.70711	0
4	2	-3.62258	-0.226301, 0.226301
6	3	-5.08036	-0.336515, 0, 0.336515
8	4	-6.61973	-0.411590, -0.101612, 0.101612, 0.411590

Table 1.1: Ground state energy and Bethe roots of the closed spin-$\frac{1}{2}$ XXZ chain in the massless regime (imaginary η), for $\eta = \frac{i\pi}{4}$.

Energy, E	degeneracy	M	shifted Bethe roots $\tilde{u}_\alpha = u_\alpha + \frac{\eta}{2}$
-3.62258	1	2	-0.226301, 0.226301
-2.0	2	1	0
		1	0
-1.41421	1	2	0 , $\frac{i\pi}{2}$
0	7	1	-0.440687
		1	-0.440687
		1	0.440687
		1	0.440687
		2	-0.329239 + $\frac{i\pi}{2}$, 0.329239
		2	0.329239 + $\frac{i\pi}{2}$, -0.329239
		2	-$\frac{\eta}{2}$, $\frac{\eta}{2}$
1.41421	2	0	-
		0	-
2.0	2	1	$\frac{i\pi}{2}$
		1	$\frac{i\pi}{2}$
2.20837	1	2	$\pm$ 0.600211 + $\frac{i\pi}{2}$

Table 1.2: Complete set of 2^4 energy levels and Bethe roots of the closed spin-$\frac{1}{2}$ XXZ chain in the massless regime, for $\eta = \frac{i\pi}{4}$.

Subsequent chapters of this dissertation consists of the following papers:

Chapter 2 "Bethe ansatz from functional relations of open XXZ chain for new special cases", JSTAT **P05007** (2005), Addendum JSTAT **P11004** (2005) and "Generalized T-Q relations and the open XXZ chain", JSTAT **P08002** (2005) by R. Murgan and R.I. Nepomechie.

Chapter 3 "Exact solution of the open XXZ chain with general integrable boundary terms at roots of unity", JSTAT **P08006** (2006) by R. Murgan, R.I. Nepomechie and Chi Shi.

Chapter 4 "Boundary energy of the open XXZ chain from new exact solutions", Annales Henri Poincare **7** (2006) 1429 by R. Murgan, R.I. Nepomechie and Chi Shi.

Chapter 5 "Boundary energy of the general open XXZ chain at roots of unity", JHEP**01** (2007) 038 by R. Murgan, R.I. Nepomechie and Chi Shi.

Chapter 6 "Finite-size correction and bulk hole-excitations for special case of an open XXZ chain with nondiagonal boundary terms at roots of unity", JHEP**05** (2007) 069 by R. Murgan.

Chapter 7 "Boundary S-matrix of an open XXZ spin chain with nondiagonal boundary terms", JHEP**03** (2008) 053 by R. Murgan.

Chapter 2: Bethe Ansatz For Special Cases of an Open XXZ Spin Chain

The open XXZ quantum spin chain with general integrable boundary terms [32] is a fundamental integrable model with boundary, which has applications in condensed matter physics, statistical mechanics and string theory. The Hamiltonian can be written as [2][6, 32]

$$\begin{aligned}\mathcal{H} &= \mathcal{H}_0 + \frac{1}{2}\sinh\eta\Big[\coth\alpha_-\tanh\beta_-\sigma_1^z + \operatorname{cosech}\alpha_-\operatorname{sech}\beta_-(\cosh\theta_-\sigma_1^x \\ &+ i\sinh\theta_-\sigma_1^y) - \coth\alpha_+\tanh\beta_+\sigma_N^z + \operatorname{cosech}\alpha_+\operatorname{sech}\beta_+(\cosh\theta_+\sigma_N^x \\ &+ i\sinh\theta_+\sigma_N^y)\Big]\,, \end{aligned} \tag{2.1}$$

where $H_{n,n+1}$ is given by

$$\mathcal{H}_0 = \frac{1}{2}\sum_{n=1}^{N-1}\left(\sigma_n^x\sigma_{n+1}^x + \sigma_n^y\sigma_{n+1}^y + \cosh\eta\ \sigma_n^z\sigma_{n+1}^z\right)\,, \tag{2.2}$$

$\sigma^x, \sigma^y, \sigma^z$ are the standard Pauli matrices, η is the bulk anisotropy parameter, $\alpha_\pm, \beta_\pm, \theta_\pm$ are arbitrary boundary parameters [3] and N is the number of spins.

Although this model remains unsolved, the special case of diagonal boundary terms was solved long ago [14, 15, 23], and some progress on the more general case has been achieved recently by two different approaches. One approach, pursued by Cao *et al.* [24] is an adaptation of the generalized algebraic Bethe Ansatz [21, 35] to open chains. Another approach, which was developed in [25]-[28] and which we pursue further here, exploits the functional relations obeyed by the transfer matrix

[2] Note that this Hamiltonian is related to the transfer matrix as encoded in (1.13)

[3] Under a global spin rotation about the z axis, the bulk terms remain invariant, and the boundary parameters $\theta_\pm$ become shifted by the same constant, $\theta_\pm \mapsto \theta_\pm + const$. Hence, the energy (and in fact, the transfer matrix eigenvalues) depend on $\theta_\pm$ only through the difference $\theta_- - \theta_+$.

at roots of unity. It is based on fusion [36], the truncation of the fusion hierarchy at roots of unity [40, 41], and the Bazhanov-Reshetikhin solution of RSOS models [37, 38]. Similar results had been known for closed spin chains [39, 40, 41].

Both approaches lead to a Bethe Ansatz solution for the special case that the boundary parameters obey a certain constraint. Namely, (following the notation of the second reference in [27] where $\alpha_- \,, \beta_- \,, \theta_-$ and $\alpha_+ \,, \beta_+ \,, \theta_+$ denote the left and right boundary parameters, respectively, and N is the number of spins in the chain),

$$\alpha_- + \beta_- + \alpha_+ + \beta_+ = \pm(\theta_- - \theta_+) + \eta k \,, \tag{2.3}$$

where k is an even integer if N is odd, and is an odd integer if N is even. See Appendix 1 for details on the Bethe Ansatz solution for this case. This solution has been used to derive a nonlinear integral equation for the sine-Gordon model on an interval [42, 43], and has been generalized to other models [44]. However, completeness of this solution is not straightforward, as two sets of Bethe Ansatz equations are generally needed in order to obtain all 2^N levels [28]. Related work includes [44]-[50].

Despite these successes, it would be desirable to find the solution for general values of the boundary parameters; i.e., when the constraint (2.3) is not satisfied. In the functional relation approach, the main difficulty lies in recasting the functional relations (which are known [26, 27] for general values of the boundary parameters) as the condition that a certain determinant vanish. In this chapter, we present the solution of this problem (and hence, the Bethe Ansatz expression for the transfer matrix eigenvalues) for the special cases that all but one of the boundary parameters are zero, and the bulk anisotropy has values $\eta = \frac{i\pi}{3} \,, \frac{i\pi}{5} \,, \ldots$. These results are extended to cases where any two of the boundary parameters $\{\alpha_-, \alpha_+, \beta_-, \beta_+\}$ are arbitrary and the remaining parameters are either η or $i\pi/2$. We also present

Bethe Ansatz solutions for cases with at most two arbitrary boundary parameters and the bulk anisotropy has values $\eta = \frac{i\pi}{2}\,, \frac{i\pi}{4}\,, \ldots$.

2.1 Transfer matrix and functional relations

The transfer matrix $t(u)$ of the open XXZ chain with general integrable boundary terms is given by (1.11). The R matrix is given by (1.2). $K^{\mp}(u)$ are 2×2 matrices whose components are given by [6, 32]

$$\begin{aligned} K^{-}_{11}(u) &= 2\left(\sinh\alpha_{-}\cosh\beta_{-}\cosh u + \cosh\alpha_{-}\sinh\beta_{-}\sinh u\right) \\ K^{-}_{22}(u) &= 2\left(\sinh\alpha_{-}\cosh\beta_{-}\cosh u - \cosh\alpha_{-}\sinh\beta_{-}\sinh u\right) \\ K^{-}_{12}(u) &= e^{\theta_{-}}\sinh 2u\,, \qquad K^{-}_{21}(u) = e^{-\theta_{-}}\sinh 2u\,, \end{aligned} \tag{2.4}$$

and

$$\begin{aligned} K^{+}_{11}(u) &= -2\left(\sinh\alpha_{+}\cosh\beta_{+}\cosh(u+\eta) - \cosh\alpha_{+}\sinh\beta_{+}\sinh(u+\eta)\right) \\ K^{+}_{22}(u) &= -2\left(\sinh\alpha_{+}\cosh\beta_{+}\cosh(u+\eta) + \cosh\alpha_{+}\sinh\beta_{+}\sinh(u+\eta)\right) \\ K^{+}_{12}(u) &= -e^{\theta_{+}}\sinh 2(u+\eta)\,, \qquad K^{+}_{21}(u) = -e^{-\theta_{+}}\sinh 2(u+\eta)\,, \end{aligned} \tag{2.5}$$

where $\alpha_{\mp}\,, \beta_{\mp}\,, \theta_{\mp}$ are the boundary parameters. [4] For $\eta \ne i\pi/2$, the first derivative of the transfer matrix at $u=0$ is related to the Hamiltonian (2.1),

$$\mathcal{H} = c_1 t'(0) + c_2 \hat{\mathbf{I}}\,, \tag{2.6}$$

where

$$\begin{aligned} c_1 &= -\left(16\sinh^{2N-1}\eta\cosh\eta\sinh\alpha_{-}\sinh\alpha_{+}\cosh\beta_{-}\cosh\beta_{+}\right)^{-1}\,, \\ c_2 &= -\frac{\sinh^2\eta + N\cosh^2\eta}{2\cosh\eta}\,. \end{aligned} \tag{2.7}$$

[4]Following [27, 28], we use a parametrization of the boundary parameters which differs from that in [6, 32]. Specifically, the matrices $K^{\mp}(u)$ are equal to those appearing in the second reference in [27] divided by the factors $\kappa_{\mp}$, respectively.

and $\hat{\mathbf{I}}$ is the identity matrix. For $u = 0$, the transfer matrix is given by

$$t(0) = c_0 \hat{\mathbf{I}}\,, \qquad c_0 = -8 \sinh^{2N} \eta \cosh \eta \sinh \alpha_- \sinh \alpha_+ \cosh \beta_- \cosh \beta_+ \,. \quad (2.8)$$

For the special case $\eta = i\pi/2$ (i.e., $p = 1$),

$$t(0) = 0\,, \qquad t'(0) = d_0 \hat{\mathbf{I}}\,, \qquad d_0 = (-1)^{N+1} 8i \sinh \alpha_- \sinh \alpha_+ \cosh \beta_- \cosh \beta_+ \quad (2.9)$$

and the Hamiltonian (2.1) is related to the second derivative of the transfer matrix at $u = 0$ [25],

$$\mathcal{H} = d_1 t''(0)\,, \qquad d_1 = (-1)^{N+1} \left(32 \sinh \alpha_- \sinh \alpha_+ \cosh \beta_- \cosh \beta_+\right)^{-1} \,. \quad (2.10)$$

In addition to the fundamental commutativity property

$$[t(u)\,, t(v)] = 0\,, \quad (2.11)$$

the transfer matrix also has $i\pi$ periodicity

$$t(u + i\pi) = t(u)\,, \quad (2.12)$$

crossing symmetry

$$t(-u - \eta) = t(u)\,, \quad (2.13)$$

and the asymptotic behavior

$$t(u) \sim -\cosh(\theta_- - \theta_+) \frac{e^{u(2N+4)+\eta(N+2)}}{2^{2N+1}} \hat{\mathbf{I}} + \ldots \qquad \text{for} \qquad u \to \infty \,. \quad (2.14)$$

For bulk anisotropy values $\eta = \frac{i\pi}{p+1}$, with $p = 1\,, 2\,, \ldots$, the transfer matrix obeys functional relations of order $p + 1$ [26, 27]

$$t(u) t(u + \eta) \ldots t(u + p\eta)$$
$$- \quad \delta(u - \eta) t(u + \eta) t(u + 2\eta) \ldots t(u + (p - 1)\eta)$$

$$
\begin{aligned}
&- \quad \delta(u)t(u+2\eta)t(u+3\eta)\ldots t(u+p\eta) \\
&- \quad \delta(u+\eta)t(u)t(u+3\eta)t(u+4\eta)\ldots t(u+p\eta) \\
&- \quad \delta(u+2\eta)t(u)t(u+\eta)t(u+4\eta)\ldots t(u+p\eta) - \ldots \\
&- \quad \delta(u+(p-1)\eta)t(u)t(u+\eta)\ldots t(u+(p-2)\eta) \\
&+ \quad \ldots = f(u)\,. \qquad (2.15)
\end{aligned}
$$

For example, for the case $p = 2$, the functional relation is

$$
\begin{aligned}
t(u)t(u+\eta)t(u+2\eta) - \delta(u-\eta)t(u+\eta) - \delta(u)t(u+2\eta) \quad &- \quad \delta(u+\eta)t(u) \\
&= \quad f(u)\,. \qquad (2.16)
\end{aligned}
$$

The functions $\delta(u)$ and $f(u)$ are given in terms of the boundary parameters $\alpha_{\mp}\,, \beta_{\mp}\,, \theta_{\mp}$ by

$$
\delta(u) = \delta_0(u)\delta_1(u)\,, \qquad f(u) = f_0(u)f_1(u)\,, \qquad (2.17)
$$

where

$$
\begin{aligned}
\delta_0(u) \quad &= \quad (\sinh u \sinh(u+2\eta))^{2N} \frac{\sinh 2u \sinh(2u+4\eta)}{\sinh(2u+\eta)\sinh(2u+3\eta)}\,, \qquad (2.18) \\
\delta_1(u) \quad &= \quad 2^4 \sinh(u+\eta+\alpha_-)\sinh(u+\eta-\alpha_-)\cosh(u+\eta+\beta_-)\cosh(u+\eta-\beta_-) \\
&\times \quad \sinh(u+\eta+\alpha_+)\sinh(u+\eta-\alpha_+)\cosh(u+\eta+\beta_+)\cosh(u+\eta-\beta_+)\,, \\
&\qquad (2.19)
\end{aligned}
$$

and therefore,

$$
\delta(u+i\pi) = \delta(u)\,, \qquad \delta(-u-2\eta) = \delta(u)\,. \qquad (2.20)
$$

For p even,

$$
f_0(u) \quad = \quad (-1)^{N+1} 2^{-2pN} \sinh^{2N}\left((p+1)u\right)\,, \qquad (2.21)
$$

$$\begin{aligned} f_1(u) &= (-1)^{N+1} 2^{3-2p} \Big(\\ & \sinh\left((p+1)\alpha_-\right) \cosh\left((p+1)\beta_-\right) \sinh\left((p+1)\alpha_+\right) \cosh\left((p+1)\beta_+\right) \\ &\times \cosh^2\left((p+1)u\right) - \cosh\left((p+1)\alpha_-\right) \sinh\left((p+1)\beta_-\right) \cosh\left((p+1)\alpha_+\right) \\ &\times \sinh\left((p+1)\beta_+\right) \sinh^2\left((p+1)u\right) - (-1)^N \cosh\left((p+1)(\theta_- - \theta_+)\right) \\ &\times \sinh^2\left((p+1)u\right) \cosh^2\left((p+1)u\right) \Big) \,. \end{aligned} \tag{2.22}$$

For p odd,

$$f_0(u) = (-1)^{N+1} 2^{-2pN} \sinh^{2N}\left((p+1)u\right) \tanh^2\left((p+1)u\right) \,, \tag{2.23}$$

$$\begin{aligned} f_1(u) &= -2^{3-2p} \Big(\\ & \cosh\left((p+1)\alpha_-\right) \cosh\left((p+1)\beta_-\right) \cosh\left((p+1)\alpha_+\right) \cosh\left((p+1)\beta_+\right) \\ &\times \sinh^2\left((p+1)u\right) - \sinh\left((p+1)\alpha_-\right) \sinh\left((p+1)\beta_-\right) \sinh\left((p+1)\alpha_+\right) \\ &\times \sinh\left((p+1)\beta_+\right) \cosh^2\left((p+1)u\right) + (-1)^N \cosh\left((p+1)(\theta_- - \theta_+)\right) \\ &\times \sinh^2\left((p+1)u\right) \cosh^2\left((p+1)u\right) \Big) \,. \end{aligned} \tag{2.24}$$

Hence, $f(u)$ satisfies

$$f(u+\eta) = f(u) \,, \qquad f(-u) = f(u) \,. \tag{2.25}$$

We also note the identity

$$f_0(u)^2 = \prod_{j=0}^{p} \delta_0(u + j\eta) \,. \tag{2.26}$$

The commutativity property (2.11) implies that the eigenvectors $|\Lambda\rangle$ of the transfer matrix $t(u)$ are independent of the spectral parameter u. Hence, the corresponding eigenvalues $\Lambda(u)$ obey the same functional relations (2.15), as well as the properties (2.12) - (2.14).

2.2 Bethe Ansatz solution: Even p, one arbitrary boundary parameter

We henceforth restrict to *even* values of p (i.e., bulk anisotropy values $\eta = \frac{i\pi}{3}, \frac{i\pi}{5}, \ldots$), and consider the various special cases that all but one of the boundary parameters are zero.

2.2.1 $\alpha_- \ne 0$

For the case that all boundary parameters are zero except for α_- (or, similarly, α_+), we find that the functional relations (2.15) for the transfer matrix eigenvalues can be written as

$$\det \mathcal{M} = 0\,, \tag{2.27}$$

where $\mathcal{M}$ is given by the $(p+1)\times(p+1)$ matrix

$$\begin{pmatrix} \Lambda(u) & -h(u) & 0 & \ldots & 0 & -h(-u+p\eta) \\ -h(-u) & \Lambda(u+p\eta) & -h(u+p\eta) & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -h(u+p^2\eta) & 0 & 0 & \ldots & -h(-u-p(p-1)\eta) & \Lambda(u+p^2\eta) \end{pmatrix} \tag{2.28}$$

(whose successive rows are obtained by simultaneously shifting $u \mapsto u + p\eta$ and cyclically permuting the columns to the right) provided that there exists a function $h(u)$ which has the properties

$$h(u+2i\pi) = h\left(u+2(p+1)\eta\right) = h(u)\,, \tag{2.29}$$

$$h(u+(p+2)\eta)\; h(-u-(p+2)\eta) = \delta(u)\,, \tag{2.30}$$

$$\prod_{j=0}^{p} h(u+2j\eta) + \prod_{j=0}^{p} h(-u-2j\eta) = f(u)\,. \tag{2.31}$$

To solve for $h(u)$, we set

$$h(u) = h_0(u) h_1(u)\,, \tag{2.32}$$

with

$$h_0(u) = (-1)^N \sinh^{2N}(u+\eta)\frac{\sinh(2u+2\eta)}{\sinh(2u+\eta)}\,. \tag{2.33}$$

Noting that

$$\begin{aligned} h_0(u+(p+2)\eta)\ h_0(-u-(p+2)\eta) &= \delta_0(u)\,, \\ \prod_{j=0}^{p} h_0(u+2j\eta) = \prod_{j=0}^{p} h_0(-u-2j\eta) &= f_0(u)\,, \end{aligned} \tag{2.34}$$

where $\delta_0(u)$ and $f_0(u)$ are given by (2.18) and (2.21), respectively, we see that $h_1(u)$ must satisfy

$$h_1(u+(p+2)\eta)\ h_1(-u-(p+2)\eta) = \delta_1(u)\,, \tag{2.35}$$

$$\prod_{j=0}^{p} h_1(u+2j\eta) + \prod_{j=0}^{p} h_1(-u-2j\eta) = f_1(u)\,. \tag{2.36}$$

Eliminating $h_1(-u-2j\eta)$ in (2.36) using (2.35), we obtain

$$z(u)^2 - z(u)f_1(u) + \prod_{j=0}^{p} \delta_1\left(u+(2j-1)\eta\right) = 0\,, \tag{2.37}$$

where

$$z(u) = \prod_{j=0}^{p} h_1(u+2j\eta)\,. \tag{2.38}$$

Solving the quadratic equation (2.37) for $z(u)$, making use of the explicit expressions (2.19) and (2.22) for $\delta_1(u)$ and $f_1(u)$, respectively, we obtain

$$\begin{aligned} z(u) &= 2^{-2(p-1)} \cosh^2\left((p+1)u\right) \sinh\left((p+1)u\right) \\ &\times \left(\sinh\left((p+1)u\right) \pm \sinh\left((p+1)\alpha_-\right)\right)\,. \end{aligned} \tag{2.39}$$

Notice that this expression for $z(u)$ has periodicity 2η, which is consistent with (2.38) and the assumed periodicity (2.29). Corresponding solutions of (2.38) for $h_1(u)$ are

$$h_1(u) = -4\cosh^2 u \sinh u \sinh(u \mp \alpha_-) \frac{\cosh\left(\frac{1}{2}(u \pm \alpha_- + \eta)\right)}{\cosh\left(\frac{1}{2}(u \mp \alpha_- - \eta)\right)}\,. \tag{2.40}$$

In short, a function $h(u)$ which satisfies (2.29) - (2.31) is given by

$$\begin{aligned} h(u) &= (-1)^{N+1} 4 \sinh^{2N}(u+\eta) \frac{\sinh(2u+2\eta)}{\sinh(2u+\eta)} \cosh^2 u \sinh u \\ &\times \sinh(u-\alpha_-) \frac{\cosh\left(\frac{1}{2}(u+\alpha_-+\eta)\right)}{\cosh\left(\frac{1}{2}(u-\alpha_--\eta)\right)}\,. \end{aligned} \tag{2.41}$$

The structure of the matrix $\mathcal{M}$ (2.28) suggests that its null eigenvector has the form $(Q(u)\,, Q(u+p\eta)\,, \ldots\,, Q(u+p^2\eta))$, where $Q(u)$ has the periodicity property

$$Q(u+2i\pi) = Q(u)\,. \tag{2.42}$$

It follows that the transfer matrix eigenvalues are given by

$$\Lambda(u) = h(u)\frac{Q(u+p\eta)}{Q(u)} + h(-u+p\eta)\frac{Q(u-p\eta)}{Q(u)}\,, \tag{2.43}$$

which evidently has the form of Baxter's TQ relation. We make the Ansatz

$$Q(u) = \prod_{j=1}^{M} \sinh\left(\frac{1}{2}(u-u_j)\right) \sinh\left(\frac{1}{2}(u+u_j-p\eta)\right)\,, \tag{2.44}$$

which has the periodicity (2.42) as well as the crossing property [5]

$$Q(-u+p\eta) = Q(u)\,. \tag{2.45}$$

The asymptotic behavior (2.14) is consistent with having M (the number of zeros u_j of $Q(u)$) given by

$$M = N + p + 1\,, \tag{2.46}$$

which we have confirmed numerically for small values of N and p. Analyticity of $\Lambda(u)$ implies the Bethe Ansatz equations

$$\frac{h(u_j)}{h(-u_j+p\eta)} = -\frac{Q(u_j-p\eta)}{Q(u_j+p\eta)}\,, \qquad j = 1\,, \ldots\,, M\,. \tag{2.47}$$

To summarize, for the special case that p is even and all boundary parameters are zero except for α_-, the eigenvalues of the transfer matrix (1.11) are given by (2.43), where $h(u)$ is given by (2.41), and $Q(u)$ is given by (2.44) and (2.46), with zeros u_j given by (2.47).

[5] Note that $\Lambda(u) = \Lambda(-u+p\eta) = \Lambda(-u-\eta)$, where the first equality follows from (2.43) and (2.45), and the second equality follows from the $i\pi$ periodicity of $\Lambda(u)$ (which, however, is not manifest from (2.43).)

We observe that for the special case that we are considering, the corresponding Hamiltonian is *not* of the usual XXZ form. Indeed, $t'(0)$ (the first derivative of the transfer matrix evaluated at $u=0$) is proportional to σ^x_N. Hence, to obtain a nontrivial integrable Hamiltonian, one must consider the second derivative of the transfer matrix. We find

$$\begin{aligned} t''(0) &= -16\sinh^{2N-1}\eta\cosh\eta\sinh\alpha_-\Bigg(\Big\{\sigma^x_N\,, \sum_{n=1}^{N-1} H_{n\,,n+1}\Big\} \\ &+ (N\cosh\eta + \sinh\eta\tanh\eta)\sigma^x_N + \frac{\sinh\eta}{\sinh\alpha_-}\sigma^x_1\sigma^x_N\Bigg)\,, \end{aligned} \tag{2.48}$$

where $H_{n\,,n+1}$ is given by

$$H_{n\,,n+1} = \frac{1}{2}\left(\sigma^x_n\sigma^x_{n+1} + \sigma^y_n\sigma^y_{n+1} + \cosh\eta\ \sigma^z_n\sigma^z_{n+1}\right)\,. \tag{2.49}$$

2.2.2 $\beta_- \neq 0$

For the case that all boundary parameters are zero except for β_- (or, similarly, β_+), we find that the functional relations (2.15) for the transfer matrix eigenvalues can again be written in the form (2.27), where now the matrix $\mathcal{M}$ is given by

$$\begin{pmatrix} \Lambda(u) & -h(u) & 0 & \dots & 0 & -h(-u-\eta) \\ -h(-u-(p+1)\eta) & \Lambda(u+p\eta) & -h(u+p\eta) & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -h(u+p^2\eta) & 0 & 0 & \dots & -h(-u-(p^2+1)\eta) & \Lambda(u+p^2\eta) \end{pmatrix} \tag{2.50}$$

if $h(u)$ satisfies

$$h(u+2i\pi) = h\left(u+2(p+1)\eta\right) = h(u)\,, \tag{2.51}$$

$$h(u+(p+2)\eta)\ h(-u-\eta) = \delta(u)\,, \tag{2.52}$$

$$\prod_{j=0}^{p} h(u+2j\eta) + \prod_{j=0}^{p} h(-u-(2j+1)\eta) = f(u)\,. \tag{2.53}$$

Proceeding similarly to the previous case, we now find

$$\begin{aligned} h(u) &= (-1)^N 4\sinh^{2N}(u+\eta)\frac{\sinh(2u+2\eta)}{\sinh(2u+\eta)}\sinh^2 u\cosh u \\ &\times \left(\cosh u + (-1)^{\frac{p}{2}} i\sinh\beta_-\right)\,. \end{aligned} \tag{2.54}$$

The transfer matrix eigenvalues are now given by

$$\Lambda(u) = h(u)\frac{Q(u+p\eta)}{Q(u)} + h(-u-\eta)\frac{Q(u-p\eta)}{Q(u)}\,, \tag{2.55}$$

with

$$Q(u) = \prod_{j=1}^{M} \sinh\left(\frac{1}{2}(u-u_j)\right) \sinh\left(\frac{1}{2}(u+u_j+\eta)\right)\,, \tag{2.56}$$

which satisfies $Q(u+2i\pi) = Q(u)$ and $Q(-u-\eta) = Q(u)$; and

$$M = N + p\,. \tag{2.57}$$

Moreover, the Bethe Ansatz equations for the zeros u_j take the form

$$\frac{h(u_j)}{h(-u_j-\eta)} = -\frac{Q(u_j-p\eta)}{Q(u_j+p\eta)}\,, \qquad j = 1\,, \ldots\,, M\,. \tag{2.58}$$

For this case, $t'(0) = 0$, and

$$t''(0) = -16\cosh\eta\,\sinh^{2N}\eta\,(\sigma_1^x + \sinh\beta_-\ \sigma_1^z)\,\sigma_N^x\,. \tag{2.59}$$

Higher derivatives yield more complicated expressions.

2.2.3 $\theta_\mp \neq 0$

For the case that all boundary parameters are zero except for θ_- and θ_+ (quantities of interest depend only on the difference $\theta_- - \theta_+$), we find that the functional relations (2.15) for the transfer matrix eigenvalues can be written in the form (2.27), where the matrix $\mathcal{M}$ is given by

$$\begin{pmatrix} \Lambda(u) & -h^{(2)}(-u-\eta) & 0 & \ldots & 0 & -h^{(1)}(u) \\ -h^{(1)}(u+\eta) & \Lambda(u+\eta) & -h^{(2)}(-u-2\eta) & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -h^{(2)}(-u-(p+1)\eta) & 0 & 0 & \ldots & -h^{(1)}(u+p\eta) & \Lambda(u+p\eta) \end{pmatrix} \tag{2.60}$$

(whose successive rows are obtained by simultaneously shifting $u \mapsto u+\eta$ and cyclically permuting the columns to the right), if the functions $h^{(1)}(u)$ and $h^{(2)}(u)$

satisfy

$$h^{(k)}(u+i\pi) = h^{(k)}\,(u+(p+1)\eta) = h^{(k)}(u)\,, \quad k=1\,,2\,, \tag{2.61}$$

$$h^{(1)}(u+\eta)\ h^{(2)}(-u-\eta) = \delta(u)\,, \tag{2.62}$$

$$\prod_{j=0}^{p} h^{(1)}(u+j\eta) + \prod_{j=0}^{p} h^{(2)}(-u-j\eta) = f(u)\,. \tag{2.63}$$

We find

$$\begin{aligned} h^{(1)}(u) &= (-1)^N e^{\theta_+-\theta_-} \sinh^{2N}(u+\eta) \frac{\sinh(2u+2\eta)}{\sinh(2u+\eta)} \sinh^2 2u\,, \\ h^{(2)}(u) &= (-1)^N e^{\theta_--\theta_+} \sinh^{2N}(u+\eta) \frac{\sinh(2u+2\eta)}{\sinh(2u+\eta)} \sinh^2 2u\,. \end{aligned} \tag{2.64}$$

The transfer matrix eigenvalues are given by

$$\Lambda(u) = h^{(1)}(u)\frac{Q(u-\eta)}{Q(u)} + h^{(2)}(-u-\eta)\frac{Q(u+\eta)}{Q(u)}\,, \tag{2.65}$$

with, for N even,

$$Q(u) = \prod_{j=1}^{2M} \sinh(u-u_j)\,, \tag{2.66}$$

which satisfies $Q(u+i\pi) = Q(u)$; and

$$M = \frac{1}{2}(N+p)\,. \tag{2.67}$$

The Bethe Ansatz equations for the zeros u_j take the form

$$\frac{h^{(1)}(u_j)}{h^{(2)}(-u_j-\eta)} = -\frac{Q(u_j+\eta)}{Q(u_j-\eta)}\,, \qquad j=1\,,\ldots\,,M\,. \tag{2.68}$$

For this case, also $t'(0)=0$, and

$$\begin{aligned} t''(0) &= -16\cosh\eta\sinh^{2N}\eta\Big(\cosh\theta_-\cosh\theta_+\ \sigma_1^x\sigma_N^x + i\cosh\theta_-\sinh\theta_+\ \sigma_1^x\sigma_N^y \\ &+ i\sinh\theta_-\cosh\theta_+\ \sigma_1^y\sigma_N^x - \sinh\theta_-\sinh\theta_+\ \sigma_1^y\sigma_N^y\Big)\,. \end{aligned} \tag{2.69}$$

2.3 Bethe Ansatz solution: Even p, two arbitrary boundary parameters

In Section 2.2, we obtained Bethe Ansatz solutions for the transfer matrix eigenvalues of the open XXZ chain for the special cases that the bulk anisotropy parameter has values

$$\eta = \frac{i\pi}{p+1}\,, \qquad p = 2\,,4\,,6\,,\ldots\,, \tag{2.70}$$

and *one* of the boundary parameters $\{\alpha_-, \alpha_+, \beta_-, \beta_+\}$ is arbitrary, and the remaining boundary parameters are zero. Here we show that those results can readily be extended to the cases that any *two* of the boundary parameters $\{\alpha_-, \alpha_+, \beta_-, \beta_+\}$ are arbitrary and the remaining boundary parameters are either η or $i\pi/2$. (We assume that $\theta_- = \theta_+ \equiv \theta$.) For these cases, the corresponding Hamiltonians have the conventional local form (see, e.g., [28])

$$\begin{aligned}
\mathcal{H} &= \sum_{n=1}^{N-1} H_{n\,,n+1} + \frac{1}{2}\sinh\eta\Big[\coth\alpha_-\tanh\beta_-\sigma_1^z \\
&+ \operatorname{cosech}\alpha_-\operatorname{sech}\beta_-(\cosh\theta\sigma_1^x + i\sinh\theta\sigma_1^y) - \coth\alpha_+\tanh\beta_+\sigma_N^z \\
&+ \operatorname{cosech}\alpha_+\operatorname{sech}\beta_+(\cosh\theta\sigma_N^x + i\sinh\theta\sigma_N^y)\Big]\,,
\end{aligned} \tag{2.71}$$

where $H_{n\,,n+1}$ is given by (2.49). The corresponding energy eigenvalues are related to the eigenvalues $\Lambda(u)$ of the transfer matrix $t(u)$ (1.11) by

$$E = c_1 \frac{\partial}{\partial u}\Lambda(u)\Big|_{u=0} + c_2\,, \tag{2.72}$$

where

$$\begin{aligned}
c_1 &= -\frac{1}{16\sinh\alpha_-\cosh\beta_-\sinh\alpha_+\cosh\beta_+\sinh^{2N-1}\eta\cosh\eta}\,, \\
c_2 &= -\frac{\sinh^2\eta + N\cosh^2\eta}{2\cosh\eta}\,.
\end{aligned} \tag{2.73}$$

2.3.1 $\alpha_-\,, \alpha_+$ arbitrary

For the case that $\alpha_\pm$ are arbitrary and $\beta_\pm = \eta$, we find that

$$\sqrt{f_1(u)^2 - 4\prod_{j=0}^{p} \delta_1\left(u + (2j-1)\eta\right)} = 2^{-2p+3}\cosh^2\left((p+1)u\right)\sinh\left((p+1)u\right) \times \Big[\sinh\left((p+1)\alpha_-\right) - (-1)^N \sinh\left((p+1)\alpha_+\right)\Big]\,. \tag{2.74}$$

The key point is that the argument of the square root is a perfect square. For definiteness, we henceforth restrict to *even* values of N. It follows that the quantity $z(u)$ appearing in (2.37) is now given by (cf. (2.39))

$$z(u) = 2^{-2(p-1)}\cosh^2\left((p+1)u\right)\left[\sinh\left((p+1)u\right) \pm \sinh\left((p+1)\alpha_-\right)\right] \times \left[\sinh\left((p+1)u\right) \mp \sinh\left((p+1)\alpha_+\right)\right]\,. \tag{2.75}$$

Corresponding solutions of (2.38) for $h_1(u)$ are (cf. (2.40))

$$h_1(u) = 4\cosh^2(u-\eta)\sinh(u\mp\alpha_-)\sinh(u\pm\alpha_+) \times \frac{\cosh\left(\frac{1}{2}(u\pm\alpha_-+\eta)\right)}{\cosh\left(\frac{1}{2}(u\mp\alpha_--\eta)\right)}\frac{\cosh\left(\frac{1}{2}(u\mp\alpha_++\eta)\right)}{\cosh\left(\frac{1}{2}(u\pm\alpha_+-\eta)\right)}\,. \tag{2.76}$$

Hence, for $h(u) = h_0(u)h_1(u)$ we can take (cf. (2.41))

$$h(u) = 4\sinh^{2N}(u+\eta)\frac{\sinh(2u+2\eta)}{\sinh(2u+\eta)}\cosh^2(u-\eta) \times \sinh(u-\alpha_-)\sinh(u+\alpha_+)\frac{\cosh\left(\frac{1}{2}(u+\alpha_-+\eta)\right)}{\cosh\left(\frac{1}{2}(u-\alpha_--\eta)\right)}\frac{\cosh\left(\frac{1}{2}(u-\alpha_++\eta)\right)}{\cosh\left(\frac{1}{2}(u+\alpha_+-\eta)\right)}\,, \tag{2.77}$$

which indeed satisfies (2.29)-(2.31). The transfer matrix eigenvalues and Bethe Ansatz equations are given by (2.43), (2.44), (2.47), with (cf. (2.46))

$$M = N + 2p + 1\,. \tag{2.78}$$

2.3.2 $\beta_-\,, \beta_+$ arbitrary

For the case that $\beta_\pm$ are arbitrary and $\alpha_\pm = \eta$, we find that

$$\sqrt{f_1(u)^2 - 4\prod_{j=0}^{p}\delta_1\left(u+(2j-1)\eta\right)} = i2^{-2p+3}\sinh^2\left((p+1)u\right)\cosh\left((p+1)u\right) \times \left[\sinh\left((p+1)\beta_-\right) - \sinh\left((p+1)\beta_+\right)\right] \tag{2.79}$$

and therefore

$$z(u) = 2^{-2(p-1)}\sinh^2\left((p+1)u\right)\left[\cosh\left((p+1)u\right) \pm i\sinh\left((p+1)\beta_-\right)\right] \times \left[\cosh\left((p+1)u\right) \mp i\sinh\left((p+1)\beta_+\right)\right]\,. \tag{2.80}$$

Thus, we take the function $h(u)$ to be (cf. (2.54))

$$h(u) = 4\sinh^{2N}(u+\eta)\frac{\sinh(2u+2\eta)}{\sinh(2u+\eta)}\sinh^2(u-\eta) \times \left(\cosh u + i\sinh\beta_-\right)\left(\cosh u - i\sinh\beta_+\right)\,, \tag{2.81}$$

which indeed satisfies (2.51)-(2.53). The transfer matrix eigenvalues and Bethe Ansatz equations are given by (2.55), (2.56), (2.58), with (cf. (2.57))

$$M = N + 2p - 1\,. \tag{2.82}$$

2.3.3 $\alpha_-\,, \beta_-$ arbitrary

For the case that $\alpha_-\,, \beta_-$ are arbitrary and $\alpha_+ = i\pi/2$, $\beta_+ = \eta$, we find that

$$\sqrt{f_1(u)^2 - 4\prod_{j=0}^{p}\delta_1\left(u+(2j-1)\eta\right)} = 2^{-2p+3}\cosh^2\left((p+1)u\right)\sinh\left((p+1)u\right) \times \left[\sinh\left((p+1)\alpha_-\right) + (-1)^{\frac{p}{2}} i\cosh\left((p+1)\beta_-\right)\right]\,, \tag{2.83}$$

and therefore

$$z(u) = 2^{-2(p-1)}\cosh^2\left((p+1)u\right)\left[\sinh\left((p+1)u\right) \pm \sinh\left((p+1)\alpha_-\right)\right] \times \left[\sinh\left((p+1)u\right) \pm (-1)^{\frac{p}{2}} i\cosh\left((p+1)\beta_-\right)\right]\,. \tag{2.84}$$

For $h(u)$ we take

$$\begin{aligned} h(u) &= 4\sinh^{2N}(u+\eta)\frac{\sinh(2u+2\eta)}{\sinh(2u+\eta)}\cosh(u-\eta)\cosh u \\ &\times \sinh(u-\alpha_-)\frac{\cosh\left(\frac{1}{2}(u+\alpha_-+\eta)\right)}{\cosh\left(\frac{1}{2}(u-\alpha_--\eta)\right)}\left(\sinh u + i\cosh\beta_-\right)\,, \end{aligned} \tag{2.85}$$

which satisfies (2.29)-(2.31). The transfer matrix eigenvalues and Bethe Ansatz equations are given by (2.43), (2.44), (2.47), with (cf. (2.46))

$$M = N + p\,. \tag{2.86}$$

Similar results hold for the case that $\alpha_+\,, \beta_+$ are arbitrary and $\alpha_- = i\pi/2$, $\beta_- = \eta$, etc.

We have checked these solutions numerically for chains of length up to $N = 6$, and have verified that they give the complete set of 2^N eigenvalues. Hence, completeness is achieved more simply than in the case that the constraint (2.3) is satisfied [28].

We emphasize that, in contrast to the solution for the case that the constraint (2.3) is satisfied, these solutions do *not* hold for generic values of the bulk anisotropy. Indeed, these solutions hold only for $\eta = \frac{i\pi}{3}\,, \frac{i\pi}{5}\,, \ldots$. Also, while the $Q(u)$ functions have periodicity $i\pi$ for the case that the constraint (2.3) is satisfied and for the case treated in Section 2.2.3, the $Q(u)$ functions have only $2i\pi$ periodicity for the cases treated in Sections 2.2.1 and 2.2.2. (See Eqs. (A1.10), (2.66), (2.44) and (2.56), respectively.)

Two key steps in our approach for solving for the function $h(u)$ (which permits the recasting of the functional relations (2.15) as the vanishing of a determinant (2.27)) are solving the quadratic equation (2.37) for $z(u)$, and factoring the result, such as in (2.38). For the special cases solved so far (namely, the case (2.3) considered in [24, 27, 28], and the new cases considered here), the discriminants of the corresponding quadratic equations are perfect squares, and the factorizations can be readily carried out. However, for general values of the boundary parameters, the discriminant is no longer a perfect square; and factoring the result becomes a formidable challenge. Perhaps elliptic functions may prove useful in this regard. [6]

2.4 Bethe Ansatz solution: Odd p, two arbitrary boundary parameters

The famous Baxter $T-Q$ relation [35], which schematically has the form

$$t(u)\ Q(u) = Q(u') + Q(u'')\,, \tag{2.87}$$

holds for many integrable models associated with the sl_2 Lie algebra and its deformations, such as the closed XXZ quantum spin chain. This relation provides one of the most direct routes to the Bethe Ansatz expression for the eigenvalues of the transfer matrix $t(u)$.

We present a generalization of this relation which involves more than one $Q(u)$,

$$\begin{aligned} t(u)\ Q_1(u) &= Q_2(u') + Q_2(u'')\,, \\ t(u)\ Q_2(u) &= Q_1(u''') + Q_1(u'''')\,. \end{aligned} \tag{2.88}$$

This structure arises naturally in the open XXZ quantum spin chain for special values of the bulk and boundary parameters. We expect that such generalized $T-Q$ relations, involving two or more independent $Q(u)$'s, may also appear in other integrable models.

We find here (again by means of the functional relations approach) that by allowing the possibility of generalized $T-Q$ relations, we can obtain Bethe-Ansatz-type expressions for the transfer matrix eigenvalues for the cases that at most *two* of the boundary parameters $\{\alpha_-, \alpha_+, \beta_-, \beta_+\}$ are nonzero, and the bulk anisotropy

[6] An attempt along this line for the case $p=1$ was considered in [25].

has values $\eta = \frac{i\pi}{2}, \frac{i\pi}{4}, \ldots$. In order to derive the generalized $T-Q$ relation, it is instructive to first understand why we are unable to obtain a conventional relation with a single $Q(u)$.

2.5 An attempt to obtain a conventional $T-Q$ relation

In order to obtain Bethe Ansatz expressions for the transfer matrix eigenvalues, we try (following [38]) to recast the functional relations as the condition that the determinant of a certain matrix vanishes. To this end, let us consider again the $(p+1)\times(p+1)$ matrix given by [27]

$$\mathcal{M}(u) = \begin{pmatrix} \Lambda(u) & -\frac{\delta(u)}{h(u+\eta)} & 0 & \ldots & 0 & -h(u) \\ -h(u+\eta) & \Lambda(u+\eta) & -\frac{\delta(u+\eta)}{h(u+2\eta)} & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -\frac{\delta(u-\eta)}{h(u)} & 0 & 0 & \ldots & -h(u+p\eta) & \Lambda(u+p\eta) \end{pmatrix} \tag{2.89}$$

where $h(u)$ is a function which is $i\pi$-periodic, but otherwise not yet specified. Evidently, successive rows of this matrix are obtained by simultaneously shifting $u \mapsto u+\eta$ and cyclically permuting the columns to the right. Hence, this matrix has the symmetry property

$$S\,\mathcal{M}(u)S^{-1} = \mathcal{M}(u+\eta)\,, \tag{2.90}$$

where S is the $(p+1)\times(p+1)$ matrix given by

$$S = \begin{pmatrix} 0 & 1 & 0 & \ldots & 0 & 0 \\ 0 & 0 & 1 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & 0 & 1 \\ 1 & 0 & 0 & \ldots & 0 & 0 \end{pmatrix}, \qquad S^{p+1} = 1\,. \tag{2.91}$$

This symmetry implies that the corresponding $T-Q$ relation would involve only one $Q(u)$. Indeed, if we assume $\det\mathcal{M}(u) = 0$ (which, as we discuss below, turns out to be false for the cases which we consider here), then $\mathcal{M}(u)$ has a null eigenvector,

$$\mathcal{M}(u)\ v(u) = 0\,. \tag{2.92}$$

The symmetry (2.90) is consistent with

$$S\ v(u) = v(u+\eta)\,, \tag{2.93}$$

which in turn implies that $v(u)$ has the form

$$v(u) = \left(Q(u)\,, Q(u+\eta)\,, \ldots\,, Q(u+p\eta)\right)\,, \qquad Q(u+i\pi) = Q(u)\,. \tag{2.94}$$

That is, all the components of $v(u)$ are determined by a single function $Q(u)$. The null eigenvector condition (2.92) together with the explicit forms (2.89), (2.94) of $\mathcal{M}(u)$ and $v(u)$ would then lead to a conventional $T-Q$ relation.

One can verify that the condition $\det \mathcal{M}(u) = 0$ indeed implies the functional relations (2.15), if $h(u)$ satisfies

$$f(u) = \prod_{j=0}^{p} h(u+j\eta) + \prod_{j=0}^{p} \frac{\delta(u+j\eta)}{h(u+j\eta)}\,. \tag{2.95}$$

Setting

$$z(u) \equiv \prod_{j=0}^{p} h(u+j\eta)\,, \tag{2.96}$$

it immediately follows from (2.95) that $z(u)$ is given by

$$z(u) = \frac{1}{2}\left(f(u) \pm \sqrt{\Delta(u)}\right)\,, \tag{2.97}$$

where $\Delta(u)$ is defined by

$$\Delta(u) \equiv f(u)^2 - 4\prod_{j=0}^{p} \delta(u+j\eta)\,. \tag{2.98}$$

We wish to focus here on new special cases that $\Delta(u)$ is a perfect square. [7] For odd values of p, $\Delta(u)$ is also a perfect square if at most *two* of the boundary

[7] When the constraint (2.3) is satisfied, $\Delta(u)$ is a perfect square; these are the cases studied in [26]. For even values of p, $\Delta(u)$ is also a perfect square if at most one of the boundary parameters is nonzero; these are the cases studied in [51].

parameters $\{\alpha_-, \alpha_+, \beta_-, \beta_+\}$ are nonzero. We henceforth restrict to such parameter values. In particular, we assume that η is given by (2.70), with p odd (i.e., bulk anisotropy values $\eta = \frac{i\pi}{2}, \frac{i\pi}{4}, \ldots$). For definiteness, here we present results for the case that $\alpha_-, \beta_- \ne 0$ and $\alpha_+ = \beta_+ = \theta_\pm = 0$. (In Section 2.6.2, we present results for the case that $\alpha_\pm \ne 0$ and $\beta_\pm = \theta_\pm = 0$; and similar results hold for the other cases.) Moreover, we also restrict to even values of N. (We expect similar results to hold for odd N.)

For such parameter values, it is easy to arrive at a contradiction. Indeed, on one hand, the definition (2.96) together with the assumed $i\pi$-periodicity of $h(u)$ (which is required for the symmetry (2.90)) imply the result $z(u) = z(u+\eta)$. On the other hand, (2.98) together with (2.17)-(2.20) and (2.23)- (2.26) imply

$$\begin{aligned}\sqrt{\Delta(u)} &= 2^{3-2p} f_0(u) \left(\cosh((p+1)\alpha_-) + \cosh((p+1)\beta_-)\right) \\ &\times \sinh^2((p+1)u) \cosh((p+1)u) \,. \end{aligned} \tag{2.99}$$

Hence, it follows from (2.97) that $z(u) \ne z(u+\eta)$, which contradicts the earlier result. We conclude that for such parameter values, it is *not* possible to find a function $h(u)$ which is $i\pi$-periodic and satisfies the condition (2.95). Hence, for such parameter values, the matrix $\mathcal{M}(u)$ given by (2.89) does *not* lead to the solution of the model, and we fail to obtain a conventional $T-Q$ relation.

We remark that if either α_+ or α_- is zero, then the Hamiltonian is no longer given by (2.1), since the coefficient c_1 (2.7) is singular. Indeed, as noted in [51], $t'(0)$ is then proportional to σ^x_N. Hence, in order to obtain a nontrivial integrable Hamiltonian, one must consider the second derivative of the transfer matrix. For the case $\alpha_-\,, \beta_- \ne 0$,

$$\begin{aligned} t''(0) &= -16 \sinh^{2N-1}\eta \cosh\eta \Bigg(\sinh\alpha_- \cosh\beta_- \left\{ \sigma^x_N \,, \sum_{n=1}^{N-1} H_{n\,,n+1} \right\} \\ &+ \sinh\alpha_- \cosh\beta_- (N\cosh\eta + \sinh\eta \tanh\eta)\sigma^x_N \end{aligned}$$

$$+ \quad \sinh\eta\, (\sigma_1^x + \sinh\beta_-\, \cosh\alpha_- \sigma_1^z)\, \sigma_N^x \Big) \,, \tag{2.100}$$

where $H_{n\,,n+1}$ is given by (2.49). The case $\alpha_\pm \ne 0$, for which the Hamiltonian instead has a conventional local form, will be discussed in the following section.

2.6 The generalized $T-Q$ relations

Instead of demanding the symmetry (2.90), let us now demand only the weaker symmetry

$$T\, \mathcal{M}(u) T^{-1} = \mathcal{M}(u+2\eta)\,, \qquad T \equiv S^2\,, \tag{2.101}$$

where S is given by (2.91). Indeed, (2.90) implies (2.101), but the converse is not true. A matrix $\mathcal{M}(u)$ with such symmetry is given by

$$\left(\begin{array}{cccccc} \Lambda(u) & -\frac{\delta(u)}{h^{(1)}(u)} & 0 & \ldots & 0 & -\frac{\delta(u-\eta)}{h^{(2)}(u-\eta)} \\ -h^{(1)}(u) & \Lambda(u+\eta) & -h^{(2)}(u+\eta) & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -h^{(2)}(u-\eta) & 0 & 0 & \ldots & -h^{(1)}(u+(p-1)\eta) & \Lambda(u+p\eta) \end{array} \right) \tag{2.102}$$

where $h^{(1)}(u)$ and $h^{(2)}(u)$ are functions which are $i\pi$-periodic, but otherwise not yet specified.

This symmetry implies that the corresponding $T-Q$ relations will involve *two* $Q(u)$'s. Indeed, assuming again that

$$\det \mathcal{M}(u) = 0\,, \tag{2.103}$$

then $\mathcal{M}(u)$ has a null eigenvector $v(u)$,

$$\mathcal{M}(u)\ v(u) = 0\,. \tag{2.104}$$

The symmetry (2.101) is consistent with

$$T\ v(u) = v(u+2\eta)\,, \tag{2.105}$$

which implies that $v(u)$ has the form

$$v(u) = \left(Q_1(u)\,, Q_2(u)\,, \ldots\,, Q_1(u-2\eta)\,, Q_2(u-2\eta) \right)\,, \tag{2.106}$$

with

$$Q_1(u) = Q_1(u+i\pi)\,, \qquad Q_2(u) = Q_2(u+i\pi)\,. \tag{2.107}$$

That is, the components of $v(u)$ are determined by *two* independent functions, $Q_1(u)$ and $Q_2(u)$. The null eigenvector condition (2.104) together with the explicit forms (2.102), (2.106) of $\mathcal{M}(u)$ and $v(u)$ now lead to generalized $T-Q$ relations,

$$\Lambda(u) = \frac{\delta(u)}{h^{(1)}(u)}\frac{Q_2(u)}{Q_1(u)} + \frac{\delta(u-\eta)}{h^{(2)}(u-\eta)}\frac{Q_2(u-2\eta)}{Q_1(u)}\,, \tag{2.108}$$

$$= h^{(1)}(u-\eta)\frac{Q_1(u-\eta)}{Q_2(u-\eta)} + h^{(2)}(u)\frac{Q_1(u+\eta)}{Q_2(u-\eta)}\,. \tag{2.109}$$

Since $\Lambda(u)$ has the crossing symmetry (2.13) and $\delta(u)$ has the crossing property (2.20), it is natural to have the two terms in (2.108) transform into each other under crossing. Hence, we set

$$h^{(2)}(u) = h^{(1)}(-u-2\eta)\,, \tag{2.110}$$

and we make the Ansatz

$$Q_1(u) = \prod_{j=1}^{M_1} \sinh(u-u_j^{(1)})\sinh(u+u_j^{(1)}+\eta)\,,$$

$$Q_2(u) = \prod_{j=1}^{M_2} \sinh(u-u_j^{(2)})\sinh(u+u_j^{(2)}+3\eta)\,, \tag{2.111}$$

which is consistent with the required periodicity (2.107) and crossing properties

$$Q_1(u) = Q_1(-u-\eta)\,, \qquad Q_2(u) = Q_2(-u-3\eta)\,. \tag{2.112}$$

Analyticity of $\Lambda(u)$ (2.108), (2.109) implies Bethe-Ansatz-type equations for the zeros $\{u_j^{(1)}\,, u_j^{(2)}\}$ of $Q_1(u)\,, Q_2(u)$, respectively,

$$\frac{\delta(u_j^{(1)})\; h^{(2)}(u_j^{(1)}-\eta)}{\delta(u_j^{(1)}-\eta)\; h^{(1)}(u_j^{(1)})} = -\frac{Q_2(u_j^{(1)}-2\eta)}{Q_2(u_j^{(1)})}\,, \qquad j = 1\,,2\,,\ldots\,,M_1\,,$$

$$\frac{h^{(1)}(u_j^{(2)})}{h^{(2)}(u_j^{(2)}+\eta)} = -\frac{Q_1(u_j^{(2)}+2\eta)}{Q_1(u_j^{(2)})}\,, \qquad j = 1\,,2\,,\ldots\,,M_2\,. \tag{2.113}$$

Note that the function $h^{(1)}(u)$ has not yet been specified, nor has the important assumption that $\mathcal{M}(u)$ has a vanishing determinant (2.103) yet been verified. These problems are closely related, and we now address them both.

One can verify that the condition $\det \mathcal{M}(u) = 0$ indeed implies the functional relations (2.15), if $h^{(1)}(u)$ satisfies

$$f(u) = w(u) \prod_{j=0,2,\ldots}^{p-1} \delta(u + j\eta) + \frac{1}{w(u)} \prod_{j=1,3,\ldots}^{p} \delta(u + j\eta) \,, \tag{2.114}$$

where

$$w(u) \equiv \frac{\prod_{j=1,3,\ldots}^{p} h^{(2)}(u + j\eta)}{\prod_{j=0,2,\ldots}^{p-1} h^{(1)}(u + j\eta)} \,. \tag{2.115}$$

It immediately follows from (2.114) that $w(u)$ is given by

$$w(u) = \frac{f(u) \pm \sqrt{\Delta(u)}}{2 \prod_{j=0,2,\ldots}^{p-1} \delta(u + j\eta)} \,, \tag{2.116}$$

where $\Delta(u)$ is the same quantity defined in (2.98).

2.6.1 $\alpha_- \neq 0$, $\beta_- \neq 0$ and $\alpha_+ = \beta_+ = \theta_\pm = 0$

We consider the case that p is odd, and that at most α_- and β_- are nonzero. For this case, $\sqrt{\Delta(u)}$ is given by (2.99). It follows from (2.116) that for $p = 3\,,7\,,11\,,\ldots$ the two solutions for $w(u)$ are given by

$$\begin{aligned} w(u) &= \coth^{2N}\left(\frac{1}{2}(p+1)u\right) \,, \\ w(u) &= \left(\frac{\cosh((p+1)u) - \cosh((p+1)\alpha_-)}{\cosh((p+1)u) + \cosh((p+1)\alpha_-)}\right)\left(\frac{\cosh((p+1)u) - \cosh((p+1)\beta_-)}{\cosh((p+1)u) + \cosh((p+1)\beta_-)}\right) \\ &\quad \times \coth^{2N}\left(\frac{1}{2}(p+1)u\right) \,, \qquad p = 3\,,7\,,11\,,\ldots\,; \end{aligned} \tag{2.117}$$

and for $p = 1\,,5\,,9\,,\ldots$ the two solutions for $w(u)$ are given by

$$\begin{aligned} w(u) &= \left(\frac{\cosh((p+1)u) - \cosh((p+1)\alpha_-)}{\cosh((p+1)u) + \cosh((p+1)\alpha_-)}\right) \coth^{2N}\left(\frac{1}{2}(p+1)u\right) \,, \\ w(u) &= \left(\frac{\cosh((p+1)u) + \cosh((p+1)\beta_-)}{\cosh((p+1)u) - \cosh((p+1)\beta_-)}\right) \coth^{2N}\left(\frac{1}{2}(p+1)u\right) \,, \\ &\quad p = 1\,,5\,,9\,,\ldots\,. \end{aligned} \tag{2.118}$$

There are many solutions of (2.115) for $h^{(1)}(u)$ (with $h^{(2)}(u)$ given by (2.110)) corresponding to the above expressions for $w(u)$, which also have the required $i\pi$ periodicity. We consider here the solutions

$$h^{(1)}(u) = -4\sinh^{2N}(u+2\eta)\,, \quad M_2 = \frac{1}{2}N + p - 1\,, \quad M_1 = M_2 + 2\,, \qquad p = 3\,,7\,,11\,,\ldots \tag{2.119}$$

and

$$h^{(1)}(u) = \begin{cases} -2\cosh(u+\alpha_-)\cosh(u-\alpha_-)\cosh(2u)\sinh^{2N}(u+2\eta)\,, \\ M_1 = M_2 = \frac{1}{2}N + 2p - 1\,, \qquad p = 9\,,17\,,25\,,\ldots \\ 2\cosh(u+\alpha_-)\cosh(u-\alpha_-)\cosh(2u)\sinh^{2N}(u+2\eta)\,, \\ M_1 = M_2 = \frac{1}{2}N + \frac{3}{2}(p-1)\,, \qquad p = 5\,,13\,,21\,,\ldots \\ 2\cosh(u+\alpha_-)\cosh(u-\alpha_-)\cosh(2u)\sinh^{2N}(u+2\eta)\,, \\ M_1 = M_2 = \frac{1}{2}N + 2\,, \qquad p = 1\,, \end{cases} \tag{2.120}$$

corresponding to the first solutions for $w(u)$ given in (2.117), (2.118), respectively. We have searched for solutions largely by trial and error, verifying numerically (along the lines explained in [28]) for small values of N that the eigenvalues can indeed be expressed as (2.108), (2.109) with $Q(u)$'s of the form (2.111).

Note that the values of M_1 and M_2 (i.e., the number of zeros of $Q_1(u)$ and $Q_2(u)$, respectively) depend on the particular choice for the function $h^{(1)}(u)$. Our reason for choosing (2.119), (2.120) over the other solutions which we found is that the former solutions gave the *lowest* values of M_1 and M_2, for given values of N and p. (It would be interesting to know whether there exist other solutions for $h^{(1)}(u)$ which give even lower values of M_1 and M_2.) Our conjectured values of M_1 and M_2 given in (2.119), (2.120) are consistent with the asymptotic behavior (2.14). Moreover, these values have been checked numerically for small values of N (up to $N = 6$) and p (up to $p = 21$). That is, we have verified numerically that, with the above choice of $h^{(1)}(u)$, the generalized $T-Q$ relations (2.108), (2.109) correctly give all 2^N eigenvalues, with $Q_1(u)$ and $Q_2(u)$ of the form (2.111) and with M_1 and M_2 given in (2.119), (2.120). We expect that similar results can be obtained corresponding to the second solutions for $w(u)$.

We propose that for the case that p is odd and that at most α_-, β_- are nonzero, the eigenvalues $\Lambda(u)$ of the transfer matrix $t(u)$ (1.11) are given by the generalized $T-Q$ relations (2.108), (2.109), with $Q_1(u)$ and $Q_2(u)$ given by (2.111), $h^{(2)}(u)$ given by (2.110), and $h^{(1)}(u)$ given by (2.119), (2.120). The zeros $\{u_j^{(1)}, u_j^{(2)}\}$ of $Q_1(u)$ and $Q_2(u)$ are solutions of the Bethe Ansatz equations (2.113). We expect that there are sufficiently many such equations to determine all the zeros. As already mentioned, similar results hold for the case that at most two of the boundary parameters $\{\alpha_-, \alpha_+, \beta_-, \beta_+\}$ are nonzero.

2.6.2 $\alpha_\pm \neq 0$ and $\beta_\pm = \theta_\pm = 0$

Here we consider the case that $\alpha_\pm \neq 0$ and $\beta_\pm = \theta_\pm = 0$, for which the Hamiltonian is local,

$$\mathcal{H} = \sum_{n=1}^{N-1} H_{n\,,n+1} + \frac{1}{2}\sinh\eta\Big(\operatorname{cosech}\alpha_-\sigma_1^x + \operatorname{cosech}\alpha_+\sigma_N^x\Big)\,, \qquad (2.121)$$

as follows from (2.1). For this case, the quantity $\sqrt{\Delta(u)}$ is given by (2.99) with β_- replaced by α_+, namely,

$$\begin{aligned}\sqrt{\Delta(u)} &= 2^{3-2p} f_0(u)\left(\cosh((p+1)\alpha_-) + \cosh((p+1)\alpha_+)\right) \\ &\times \sinh^2((p+1)u)\cosh((p+1)u)\,. \end{aligned} \qquad (2.122)$$

It follows that the two solutions for $w(u)$ (2.116) are given by

$$\begin{aligned} w(u) &= \coth^{2N}\left(\frac{1}{2}(p+1)u\right)\,, \\ w(u) &= \left(\frac{\cosh((p+1)u) - \cosh((p+1)\alpha_-)}{\cosh((p+1)u) + \cosh((p+1)\alpha_-)}\right)\left(\frac{\cosh((p+1)u) - \cosh((p+1)\alpha_+)}{\cosh((p+1)u) + \cosh((p+1)\alpha_+)}\right) \\ &\times \coth^{2N}\left(\frac{1}{2}(p+1)u\right)\,, \qquad p = 3\,,7\,,11\,,\ldots\,, \end{aligned} \qquad (2.123)$$

and

$$
\begin{aligned}
w(u) &= \coth^{2N+2}\left(\frac{1}{2}(p+1)u\right) , \\
w(u) &= \left(\frac{\cosh((p+1)u) - \cosh((p+1)\alpha_-)}{\cosh((p+1)u) + \cosh((p+1)\alpha_-)}\right)\left(\frac{\cosh((p+1)u) - \cosh((p+1)\alpha_+)}{\cosh((p+1)u) + \cosh((p+1)\alpha_+)}\right) \\
&\quad \times \coth^{2N+2}\left(\frac{1}{2}(p+1)u\right) , \qquad p = 1 , 5 , 9 , \ldots . \qquad (2.124)
\end{aligned}
$$

For simplicity, let us once again consider just the first solutions for $w(u)$ given in (2.123) and (2.124), which are independent of $\alpha_\pm$. Corresponding solutions of (2.115) for $h^{(1)}(u)$ (with $h^{(2)}(u)$ given by (2.110)) are

$$
h^{(1)}(u) = 4\sinh^{2N}(u+2\eta) , \quad M_2 = \frac{1}{2}N + \frac{1}{2}(3p-1) , \quad M_1 = M_2 + 2 , \qquad p = 3 , 7 , 11 , \ldots \quad (2.125)
$$

and

$$
h^{(1)}(u) = \begin{cases} -2\cosh(2u)\sinh^2 u \sinh^{2N}(u+2\eta) , & M_1 = M_2 = \frac{1}{2}N + 2p - 1 , \\ \qquad p = 9 , 17 , 25 , \ldots & \\ 2\cosh(2u)\sinh^2 u \sinh^{2N}(u+2\eta) , & M_1 = M_2 = \frac{1}{2}N + \frac{3}{2}(p-1) , \\ \qquad p = 5 , 13 , 21 , \ldots & \\ 2\cosh(2u)\sinh^2 u \sinh^{2N}(u+2\eta) , & M_1 = M_2 = \frac{1}{2}N + 2 , \\ \qquad p = 1 . & \end{cases} \qquad (2.126)
$$

That is, the eigenvalues $\Lambda(u)$ of the transfer matrix $t(u)$ (1.11), for η values (2.70) with p odd and for $\alpha_\pm \ne 0$ and $\beta_\pm = \theta_\pm = 0$, are given by the generalized $T-Q$ relations (2.108), (2.109), with $Q_1(u)$ and $Q_2(u)$ given by (2.111), $h^{(2)}(u)$ given by (2.110), and $h^{(1)}(u)$ given by (2.125), (2.126). The zeros $\{u_j^{(1)} , u_j^{(2)}\}$ of $Q_1(u)$ and $Q_2(u)$ are solutions of the Bethe Ansatz equations (2.113).

We have argued that the eigenvalues of the transfer matrix of the open XXZ chain, for the special case that p is odd and that at most two of the boundary parameters $\{\alpha_-, \alpha_+, \beta_-, \beta_+\}$ are nonzero, can be given by generalized $T-Q$ relations (2.108), (2.109) involving more than one $Q(u)$. Although we have not ruled out the possibility of expressing these eigenvalues in terms of a conventional $T-Q$ relation, the analysis in Section 2.5 suggests to us that this is unlikely.

It should be possible to explicitly construct *operators* $Q_1(u)$, $Q_2(u)$ which commute with each other and with the transfer matrix $t(u)$, and whose eigenvalues are given by (2.111). There may be further special cases for which the quantity $\Delta(u)$ (2.98) is a perfect square, in which case it should not be difficult to find the corresponding Bethe Ansatz solution. The general case that $\Delta(u)$ is *not* a perfect square and/or that $\eta \neq i\pi/(p+1)$ remains to be understood.

Generalized $T-Q$ relations are novel structures, which merit further investigation. The corresponding Bethe Ansatz equations (e.g., (2.113)) have some resemblance to the "nested" equations which are characteristic of higher-rank models. Such generalized $T-Q$ relations, involving two or even more $Q(u)$'s, may also lead to further solutions of integrable open chains of higher rank and/or higher-dimensional representations. (For recent progress on such models, see e.g. [44].)

Chapter 3: Bethe Ansatz For General Case of an Open XXZ Spin Chain

There remains the vexing problem of solving the model when the constraint (2.3) is *not* satisfied, i.e., for *arbitrary* values of the boundary parameters. Our goal has been to solve this problem for the root of unity case. Some progress was already achieved in [51, 52], where Bethe-Ansatz-type solutions for special cases with up to two free boundary parameters (and with the remaining boundary parameters fixed to specific values) were proposed. For those special cases (as well as for the cases where the constraint (2.3) is satisfied), the quantity $\Delta(u)$ defined by (2.98), namely

$$\Delta(u) = f(u)^2 - 4 \prod_{j=0}^{p} \delta(u + j\eta) \tag{3.1}$$

is a perfect square. However, for generic values of boundary parameters, $\Delta(u)$ is *not* a perfect square, and it had not been clear to us how to proceed. It is on this generic case that we focus in this chapter.

We find, for generic values of the boundary parameters, expressions for the eigenvalues $\Lambda(u)$ of the transfer matrix $t(u)$ in terms of sets of "Q functions" $\{a_i(u)\,, b_i(u)\}$, whose zeros are given by Bethe-Ansatz-like equations. (See (3.42), (3.43) for $p > 1$; and (3.69), (3.70) for $p = 1$.) Such *generalized* $T - Q$ relations, involving more than one Q function, appeared already for certain special cases [52], and were used in [53] to compute the corresponding boundary energies in the thermodynamic limit. We have verified the $T - Q$ relations numerically for small values of p and N, and confirmed that they describe the complete set of 2^N eigenvalues.

3.1 The case $p > 1$

We treat in this section the case $\eta = i\pi/(p+1)$ with $p > 1$, i.e., bulk anisotropy values $\eta = \frac{i\pi}{3}, \frac{i\pi}{4}, \ldots$. Following Bazhanov and Reshetikhin [38], we first recast the functional relations for the transfer matrix eigenvalues $\Lambda(u)$ as the condition that a matrix $\mathcal{M}(u)$ have zero determinant. The equations for the corresponding null eigenvector, together with a key Ansatz (3.38)-(3.39), then lead to the desired set of generalized $T-Q$ relations for $\Lambda(u)$ (3.42), (3.43) and the associated Bethe-Ansatz equations (3.45)-(3.52).

3.1.1 The matrix $\mathcal{M}(u)$

Our objective is to determine the eigenvalues $\Lambda(u)$ of the transfer matrix $t(u)$. As noted earlier, the transfer matrix satisfies a functional relation (2.15). By virtue of the commutativity property (2.11), the eigenvalues satisfy the same functional relation as the corresponding transfer matrix, as well as the properties (2.12) - (2.14). Hence, for example, for $p = 2$ the eigenvalues satisfy

$$\begin{aligned} \Lambda(u)\ \Lambda(u+\eta)\ \Lambda(u+2\eta) \ &- \ \delta(u)\ \Lambda(u+2\eta) - \delta(u+\eta)\ \Lambda(u) \\ &- \ \delta(u+2\eta)\ \Lambda(u+\eta) = f(u)\,. \end{aligned} \tag{3.2}$$

The first main step is to reformulate the functional relation as the condition that the determinant of some matrix vanish. To this end, let us consider the $(p+1)\times(p+1)$ matrix $\mathcal{M}(u)$ given by

$$\begin{pmatrix} \Lambda(u) & -m_1(u) & 0 & \ldots & 0 & 0 & -n_{p+1}(u) \\ -n_1(u) & \Lambda(u+\eta) & -m_2(u) & \ldots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & -n_{p-1}(u) & \Lambda(u+(p-1)\eta) & -m_p(u) \\ -m_{p+1}(u) & 0 & 0 & \ldots & 0 & -n_p(u) & \Lambda(u+p\eta) \end{pmatrix} \tag{3.3}$$

where the matrix elements $\{m_j(u)\,, n_j(u)\}$ are still to be determined. Evidently, this matrix is essentially tridiagonal, with nonzero elements also in the lower left and upper right corners. One can verify that in order to recast the functional relations as

$$\det \mathcal{M}(u) = 0\,, \tag{3.4}$$

it is sufficient that the off-diagonal matrix elements $\{m_j(u)\,, n_j(u)\}$ be periodic functions of u with period $i\pi$, and satisfy the conditions

$$\begin{aligned} m_j(u)\; n_j(u) &= \delta(u+(j-1)\eta)\,, \qquad j = 1\,, 2\,, \ldots\,, p+1\,, & (3.5)\\ \prod_{j=1}^{p+1} m_j(u) + \prod_{j=1}^{p+1} n_j(u) &= f(u)\,. & (3.6)\end{aligned}$$

We now proceed to determine a set of off-diagonal matrix elements $\{m_j(u)\,, n_j(u)\}$ which satisfies these conditions. Using (3.5) to express $n_j(u)$ in terms of $m_j(u)$, and then substituting into (3.6), we immediately see that the quantity $z(u) \equiv \prod_{j=1}^{p+1} m_j(u)$ must satisfy

$$z(u) + \frac{1}{z(u)} \prod_{j=0}^{p} \delta(u+j\eta) = f(u)\,. \tag{3.7}$$

This being a quadratic equation for $z(u)$, we readily obtain the two solutions

$$z^{\pm}(u) = \frac{1}{2}\left(f(u) \pm \sqrt{\Delta(u)}\right)\,, \tag{3.8}$$

where the discriminant $\Delta(u)$ is the quantity (2.98),

$$\Delta(u) = f(u)^2 - 4\prod_{j=0}^{p} \delta(u+j\eta)\,. \tag{3.9}$$

In short, we must find a set of matrix elements $\{m_j(u)\,, n_j(u)\}$ which satisfies (3.5) and also

$$\prod_{j=1}^{p+1} m_j(u) = z^{\pm}(u)\,, \tag{3.10}$$

where $z^{\pm}(u)$ is given by (3.8).

In previous work [27, 51, 52] we considered special cases for which $\Delta(u)$ is a perfect square. However, for generic values of the boundary parameters, $\Delta(u)$

is *not* a perfect square. Hence, the off-diagonal matrix elements *cannot* all be meromorphic functions of u.

In order to determine these matrix elements, it is convenient to recast the expression for $z^{\pm}(u)$ into a more manageable form. Noting that (see (2.18), (2.21) and (2.23))

$$\prod_{j=0}^{p} \delta_0(u+j\eta) = f_0(u)^2 \,, \tag{3.11}$$

we see that

$$\Delta(u) = f_0(u)^2 \; \Delta_1(u) \,, \tag{3.12}$$

where we have defined

$$\Delta_1(u) = f_1(u)^2 - 4 \prod_{j=0}^{p} \delta_1(u+j\eta) \,. \tag{3.13}$$

It follows from (3.8) and (3.12) that

$$z^{\pm}(u) = f_0(u) \; z_1^{\pm}(u) \,, \tag{3.14}$$

where

$$z_1^{\pm}(u) = \frac{1}{2}\left(f_1(u) \pm \sqrt{\Delta_1(u)}\right) \,. \tag{3.15}$$

Using the explicit expressions for $\delta_1(u)$ (2.19) and $f_1(u)$ (2.22), (2.24), one can show that $\Delta_1(u)$ (3.13) can be expressed as

$$\Delta_1(u) = 4\sinh^2(2(p+1)u) \sum_{k=0}^{2} \mu_k \cosh^k(2(p+1)u) \,, \tag{3.16}$$

where the coefficients μ_k, which depend on the boundary parameters, are given in the Appendix (A2.1), (A2.2) for even and odd values of p, respectively. It follows from (3.15) and (3.16) that

$$z_1^{\pm}(u) = \frac{1}{2}\left(f_1(u) \pm g_1(u)\; Y(u)\right) \,, \tag{3.17}$$

where we have defined

$$g_1(u) = 2\sinh(2(p+1)u) \tag{3.18}$$

and

$$Y(u) = \sqrt{\sum_{k=0}^{2} \mu_k \cosh^k(2(p+1)u)}\,, \tag{3.19}$$

which we take to be a single-valued continuous branch obtained by introducing suitable branch cuts in the complex u plane.[8] One can see that $Y(u)$ has the properties

$$Y(u+\eta) = Y(u)\,, \qquad Y(-u) = Y(u)\,. \tag{3.20}$$

It follows from (2.25), (3.17) and (3.18) that

$$z_1^{\pm}(u+\eta) = z_1^{\pm}(u) \qquad z_1^{+}(-u) = z_1^{-}(u)\,. \tag{3.21}$$

In short, $z^{\pm}(u)$ is given by (3.14), where $z_1^{\pm}(u)$ is given by (3.17) - (3.19), and has the important properties (3.21).

In order to construct the desired set of matrix elements, it is also convenient to introduce the function $h(u)$,

$$h(u) = h_0(u)\ h_1(u)\,, \tag{3.22}$$

where $h_0(u)$ is given by

$$h_0(u) = (-1)^N \sinh^{2N}(u+\eta)\frac{\sinh(2u+2\eta)}{\sinh(2u+\eta)}\,, \tag{3.23}$$

and satisfies

$$h_0(u)\ h_0(-u) \quad = \quad \delta_0(u-\eta)\,, \tag{3.24}$$

$$\prod_{k=0}^{p} h_0(u+k\eta) = \prod_{k=0}^{p} h_0(-u-k\eta) \quad = \quad f_0(u)\,. \tag{3.25}$$

[8] We assume that the boundary parameters have generic values, and therefore, the function $\sum_{k=0}^{2} \mu_k \cosh^k(2(p+1)u)$ is not a perfect square. The branch points are zeros of this function.

Moreover, $h_1(u)$ is given by [9]

$$h_1(u) = (-1)^{N+1} 4 \sinh(u+\alpha_-)\cosh(u+\beta_-)\sinh(u+\alpha_+)\cosh(u+\beta_+)\,, \tag{3.26}$$

and satisfies

$$h_1(u)\ h_1(-u) = \delta_1(u-\eta)\,. \tag{3.27}$$

We are finally ready to explicitly construct the requisite matrix elements:

$$\begin{aligned} m_j(u) &= h(-u-j\eta)\,, \qquad n_j(u) = h(u+j\eta)\,, \qquad j = 1\,,2\,,\ldots\,,p\,, \\ m_{p+1}(u) &= \frac{z^-(u)}{\prod_{k=1}^p h(-u-k\eta)} = \frac{z_1^-(u)\ h_0(-u)}{\prod_{k=1}^p h_1(-u-k\eta)}\,, \\ n_{p+1}(u) &= \frac{z^+(u)}{\prod_{k=1}^p h(u+k\eta)} = \frac{z_1^+(u)\ h_0(u)}{\prod_{k=1}^p h_1(u+k\eta)}\,, \end{aligned} \tag{3.28}$$

Indeed, using (3.24), (3.27) and the fact

$$z^+(u)\ z^-(u) = \prod_{j=0}^p \delta(u+j\eta) \tag{3.29}$$

(which follows from (3.8) and (3.9)), it is easy to see that the condition (3.5) is satisfied. It is also easy to see that the condition (3.10) (with $z^-(u)$ on the RHS) is also satisfied. We note here for future reference that

$$n_{p+1}(u) = m_{p+1}(-u)\,, \tag{3.30}$$

which follows from (3.21). We also note that if the constraint (2.3) with $\epsilon_1 = \epsilon_2 = \epsilon_3 = 1$ is satisfied, then $\prod_{k=0}^p h_1(u+k\eta) = z_1^\pm(u)$, as follows from the identity (A1.8). Hence, for this case, $n_{p+1}(u) = h(u)$, and the matrix $\mathcal{M}(u)$ reduces to the one considered in [27].

[9]Presumably, one can use the more general expression $h_1(u) = (-1)^{N+1} 4 \sinh(u+\alpha_-)\cosh(u+\epsilon_1\beta_-)\sinh(u+\epsilon_2\alpha_+)\cosh(u+\epsilon_3\beta_+)$, where $\epsilon_i = \pm 1$, which also satisfies (3.27). However, for simplicity, we restrict to the special case $\epsilon_i = 1$.

3.1.2 Bethe Ansatz

The fact (3.4) that $\mathcal{M}(u)$ has a zero determinant implies that it has a null eigenvector $v(u) = (v_1(u)\,, v_2(u)\,, \ldots\,, v_{p+1}(u))$,

$$\mathcal{M}(u)\ v(u) = 0\,. \tag{3.31}$$

We shall assume the periodicity

$$v_j(u + i\pi) = v_j(u + (p+1)\eta) = v_j(u)\,, \qquad j = 1\,, \ldots\,, p+1\,, \tag{3.32}$$

which is consistent with the periodicity $\mathcal{M}(u+i\pi) = \mathcal{M}(u)$. It follows from (3.31) and the expression (3.3) for $\mathcal{M}(u)$ that

$$\Lambda(u + (j-1)\eta)\ v_j(u) = n_{j-1}(u)\ v_{j-1}(u) + m_j(u)\ v_{j+1}(u)\,, \qquad j = 1\,, 2\,, \ldots\,, p+1\,, \tag{3.33}$$

where $v_{j+p+1} = v_j$ and $n_{j+p+1} = n_j$. Shifting $u \mapsto u - (j-1)\eta$, we readily obtain

$$\begin{aligned} \Lambda(u)\ v_1(u) &= h(-u-\eta)\ v_2(u) + n_{p+1}(u)\ v_{p+1}(u)\,, \\ \Lambda(u)\ v_j(u-(j-1)\eta) &= h(u)\ v_{j-1}(u-(j-1)\eta) + h(-u-\eta)\ v_{j+1}(u-(j-1)\eta)\,, \\ &\qquad j = 2\,, 3\,, \ldots\,, p\,, \\ \Lambda(u)\ v_{p+1}(u-p\eta) &= h(u)\ v_p(u-p\eta) + m_{p+1}(u-p\eta)\ v_1(u-p\eta)\,. \end{aligned} \tag{3.34}$$

The crossing properties of the eigenvalue $\Lambda(-u-\eta) = \Lambda(u)$ (2.13) together with (3.30) suggest a corresponding crossing property of $v(u)$, namely,

$$v_j(-u) = v_{p+2-j}(u)\,, \qquad j = 1\,, 2\,, \ldots\,, p+1\,. \tag{3.35}$$

In particular, for $j = \frac{p}{2} + 1$ (which occurs only for p even !), this relation implies that $v_{\frac{p}{2}+1}(u)$ is crossing invariant,

$$v_{\frac{p}{2}+1}(-u) = v_{\frac{p}{2}+1}(u)\,. \tag{3.36}$$

Moreover, (3.35) implies that at most $\lfloor \frac{p}{2} \rfloor + 1$ components of $v(u)$ are independent, say, $\{ v_1(u) \,, \ldots \,, v_{\lfloor \frac{p}{2} \rfloor + 1}(u) \}$, where $\lfloor \quad \rfloor$ denotes integer part.

Substituting the explicit expression for $n_{p+1}(u)$ (3.28) into (3.34), we obtain the relations

$$\begin{aligned} \Lambda(u)\ v_1(u) &= h(-u-\eta)\ v_2(u) + \frac{z_1^+(u)\ h_0(u)}{\prod_{k=1}^{p} h_1(u+k\eta)}\ v_1(-u) \,, \\ \Lambda(u)\ v_j(u-(j-1)\eta) &= h(u)\ v_{j-1}(u-(j-1)\eta) + h(-u-\eta)\ v_{j+1}(u-(j-1)\eta) \,, \\ & \qquad j = 2 \,, \ldots \,, \lfloor \frac{p}{2} \rfloor + 1 \,, \end{aligned} \tag{3.37}$$

which evidently resemble a system of generalized $T-Q$ equations. However, since $\Lambda(u)$ is an analytic function of u for finite values of u [10], the functions $v_j(u)$ *cannot* be analytic due to the presence of the $z_1^+(u)$ factor in (3.37).

We therefore propose instead the following Ansatz:

$$v_j(u) = a_j(u) + b_j(u)\ Y(u) \,, \qquad j = 1 \,, 2 \,, \ldots \,, \lfloor \frac{p}{2} \rfloor + 1 \,, \tag{3.38}$$

where $Y(u)$ is the function (3.19), and $a_j(u) \,, b_j(u)$ are periodic, analytic functions of u,

$$\begin{aligned} a_j(u) &= A_j \prod_{k=1}^{2M_a} \sinh(u - u_k^{(a_j)}) \,, \quad b_j(u) = B_j \prod_{k=1}^{2M_b} \sinh(u - u_k^{(b_j)}) \,, \qquad j \ne \frac{p}{2} + 1 \,, \\ a_{\frac{p}{2}+1}(u) &= A_{\frac{p}{2}+1} \prod_{k=1}^{M_a} \sinh(u - u_k^{(a_{\frac{p}{2}+1})}) \sinh(u + u_k^{(a_{\frac{p}{2}+1})}) \,, \\ b_{\frac{p}{2}+1}(u) &= B_{\frac{p}{2}+1} \prod_{k=1}^{M_b} \sinh(u - u_k^{(b_{\frac{p}{2}+1})}) \sinh(u + u_k^{(b_{\frac{p}{2}+1})}) \,, \end{aligned} \tag{3.39}$$

whose zeros $\{ u_k^{(a_j)} \,, u_k^{(b_j)} \}$, normalization constants $\{ A_j \,, B_j \}$, and also the integers $M_a \,, M_b$ are still to be determined. [11] The forms (3.39) for $a_j(u)$ and $b_j(u)$ evidently have the periodicity and crossing properties

$$a_j(u + i\pi) = a_j(u) \,, \qquad b_j(u + i\pi) = b_j(u) \,, \qquad j = 1 \,, \ldots \,, p+1 \,,$$

[10] This is a well-known consequence of the transfer matrix properties (2.11) - (2.14).

[11] Since the normalization of the null eigenvector $v(u)$ is arbitrary, one of the normalization constants, say B_1, can be set to unity.

$$a_{\frac{p}{2}+1}(-u) \;=\; a_{\frac{p}{2}+1}(u)\,, \qquad b_{\frac{p}{2}+1}(-u) = b_{\frac{p}{2}+1}(u)\,, \tag{3.40}$$

which reflect the corresponding properties of $v_j(u)$ (3.32), (3.36) and of $Y(u)$ (3.20). We have obtained numerical support for this Ansatz, which we discuss at the end of this section.

We now substitute the Ansatz (3.38), as well as the expression for $z_1^+(u)$ (3.17), into (3.37). Since $\Lambda(u)$ and $Y(u)^2$ (but not $Y(u)$!) are analytic function of u, we can separately equate the terms that are linear in $Y(u)$, and the terms with even (i.e., 0 or 2) powers of $Y(u)$. In this way we finally arrive at the generalized $T-Q$ equations:

$$\begin{aligned}\Lambda(u)\ a_1(u) \ &= h(-u-\eta)\ a_2(u) \ + \ \frac{h_0(u)}{2\prod_{k=1}^{p} h_1(u+k\eta)}\Big[f_1(u)\ a_1(-u) \\ &\quad + \ g_1(u)\ Y(u)^2\ b_1(-u)\Big]\,,\end{aligned} \tag{3.41}$$

$$\begin{aligned}\Lambda(u)\ a_j(u-(j-1)\eta) \;&=\; h(u)\ a_{j-1}(u-(j-1)\eta) + h(-u-\eta)\ a_{j+1}(u-(j-1)\eta)\,, \\ & j = 2\,, \ldots\,, \lfloor \frac{p}{2} \rfloor + 1\,,\end{aligned} \tag{3.42}$$

and

$$\Lambda(u)\ b_1(u) \ = h(-u-\eta)\ b_2(u) + \frac{h_0(u)}{2\prod_{k=1}^{p} h_1(u+k\eta)}\Big[f_1(u)\ b_1(-u) + g_1(u)\ a_1(-u)\Big]\,,$$

$$\begin{aligned}\Lambda(u)\ b_j(u-(j-1)\eta) \;&=\; h(u)\ b_{j-1}(u-(j-1)\eta) + h(-u-\eta)\ b_{j+1}(u-(j-1)\eta)\,, \\ & j = 2\,, \ldots\,, \lfloor \frac{p}{2} \rfloor + 1\,,\end{aligned} \tag{3.43}$$

where $a_{\frac{p}{2}+2}(u) = a_{\frac{p}{2}}(-u)$ and $a_{\frac{p+3}{2}}(u) = a_{\frac{p+1}{2}}(-u)$ for even and odd values of p, respectively, and similarly for the b's.

The asymptotic behavior $\Lambda(u) \sim e^{u(2N+4)}$ for $u \to \infty$ (2.14) together with the $T-Q$ equations imply the relation

$$M_a = M_b + p + 1\,. \tag{3.44}$$

An analysis of the u-independent terms yields relations among the normalization constants and sums of zeros ($\sum_l u_l^{(a_j)}\,, \sum_l u_l^{(b_j)}$), which we do not record here.

As usual, analyticity of $\Lambda(u)$ and the $T-Q$ equations imply Bethe-Ansatz-like equations for the zeros $\{u_l^{(a_j)}\}$ of the functions $\{a_j(u)\}$,

$$\begin{aligned}\frac{h_0(-u_l^{(a_1)}-\eta)}{h_0(u_l^{(a_1)})} &= -\frac{f_1(u_l^{(a_1)})\ a_1(-u_l^{(a_1)}) + g_1(u_l^{(a_1)})\ Y(u_l^{(a_1)})^2\ b_1(-u_l^{(a_1)})}{2a_2(u_l^{(a_1)})\ h_1(-u_l^{(a_1)}-\eta)\ \prod_{k=1}^{p} h_1(u_l^{(a_1)}+k\eta)}\,, \\ \frac{h(-u_l^{(a_j)}-j\eta)}{h(u_l^{(a_j)}+(j-1)\eta)} &= -\frac{a_{j-1}(u_l^{(a_j)})}{a_{j+1}(u_l^{(a_j)})}\,, \qquad j=2\,,\ldots\,,\lfloor\frac{p}{2}\rfloor+1\,, \end{aligned} \tag{3.45}$$

and for the zeros $\{u_l^{(b_j)}\}$ of the functions $\{b_j(u)\}$,

$$\begin{aligned}\frac{h_0(-u_l^{(b_1)}-\eta)}{h_0(u_l^{(b_1)})} &= -\frac{f_1(u_l^{(b_1)})\ b_1(-u_l^{(b_1)}) + g_1(u_l^{(b_1)})\ a_1(-u_l^{(b_1)})}{2b_2(u_l^{(b_1)})\ h_1(-u_l^{(b_1)}-\eta)\ \prod_{k=1}^{p} h_1(u_l^{(b_1)}+k\eta)}\,, \\ \frac{h(-u_l^{(b_j)}-j\eta)}{h(u_l^{(b_j)}+(j-1)\eta)} &= -\frac{b_{j-1}(u_l^{(b_j)})}{b_{j+1}(u_l^{(b_j)})}\,, \qquad j=2\,,\ldots\,,\lfloor\frac{p}{2}\rfloor+1\,. \end{aligned} \tag{3.46}$$

Moreover, there are additional Bethe-Ansatz-like equations for the normalization constants. Indeed, noting that $h_0(u)$ has a pole at $u=-\frac{\eta}{2}$, it follows from the analyticity of $\Lambda(u)$ and the $T-Q$ equations (3.42) that

$$a_1(\frac{\eta}{2}) = a_2(-\frac{\eta}{2})\,, \tag{3.47}$$

$$a_{j-1}((\frac{1}{2}-j)\eta) = a_{j+1}((\frac{1}{2}-j)\eta)\,, \qquad j=2\,,\ldots\,,\lfloor\frac{p}{2}\rfloor+1\,. \tag{3.48}$$

In obtaining the first equation (3.47), we have made use of the identity

$$f_1(-\frac{\eta}{2}) = 2\prod_{k=0}^{p} h_1(-\frac{\eta}{2}+\eta k)\,. \tag{3.49}$$

The equations (3.47), (3.48) evidently further relate the normalization constants $\{A_j\}$. Similarly, the $T-Q$ equations (3.43) imply

$$b_1(\frac{\eta}{2}) = b_2(-\frac{\eta}{2})\,, \tag{3.50}$$

$$b_{j-1}((\frac{1}{2}-j)\eta) = b_{j+1}((\frac{1}{2}-j)\eta)\,, \qquad j=2\,,\ldots\,,\lfloor\frac{p}{2}\rfloor+1\,, \tag{3.51}$$

which relate the normalization constants $\{B_j\}$. Finally, noting that the first (i.e., $j = 1$) $T - Q$ equation in the set (3.43) has the factor $\prod_{k=1}^{p} h_1(u + k\eta)$ in the denominator which can vanish, e.g. at $u = -\alpha_- - \eta$, leads to the relation

$$f_1(-\alpha_- - \eta)\; b_1(\alpha_- + \eta) = -g_1(-\alpha_- - \eta)\; a_1(\alpha_- + \eta)\,, \tag{3.52}$$

which relates the normalization constants A_1 and B_1. A similar analysis of the first equation in (3.42) gives an equivalent result, by virtue of the identity $f_1(u_0)^2 = g_1(u_0)^2 Y(u_0)^2$ if u_0 satisfies $\prod_{j=0}^{p} \delta_1(u_0 + j\eta) = 0$, which follows from (3.13) and the fact (3.16) that $\Delta_1(u) = g_1(u)^2 Y(u)^2$.

The energy eigenvalues of the Hamiltonian (2.1) follow from (2.6)-(2.8) and the $T - Q$ relations (3.42),

$$E = c_1 \Lambda'(0) + c_2 = c_1 c_0 \left[-\frac{a_j'(-(j-1)\eta)}{a_j(-(j-1)\eta)} + \frac{a_{j-1}'(-(j-1)\eta)}{a_{j-1}(-(j-1)\eta)} + \frac{h'(0)}{h(0)} \right] + c_2 \tag{3.53}$$

where j can take any value in the set $\{2\,, \ldots\,, \lfloor \frac{p}{2} \rfloor + 1\}$. For $j \neq \frac{p}{2} + 1$, it follows that

$$\begin{aligned} E &= \frac{1}{2} \sinh\eta \sum_{l=1}^{2M_a} \left[\coth(u_l^{(a_j)} + (j-1)\eta) - \coth(u_l^{(a_{j-1})} + (j-1)\eta) \right] \\ &+ \frac{1}{2} \sinh\eta \left(\coth\alpha_- + \tanh\beta_- + \coth\alpha_+ + \tanh\beta_+ \right) + \frac{1}{2}(N-1)\cosh\eta\,, \end{aligned} \tag{3.54}$$

which does not depend explicitly on the normalization constants. For $j = \frac{p}{2} + 1$, there is an additional contribution from the term $\frac{a_j'(-(j-1)\eta)}{a_j(-(j-1)\eta)}$ in (3.53), since this $a_j(u)$ is crossing invariant. It follows that

$$\begin{aligned} E &= \frac{1}{2} \sinh\eta \\ &\times \left\{ \sum_{l=1}^{M_a} \left[\coth(u_l^{(a_{\frac{p}{2}+1})} + \frac{p\eta}{2}) - \coth(u_l^{(a_{\frac{p}{2}+1})} - \frac{p\eta}{2}) \right] - \sum_{l=1}^{2M_a} \coth(u_l^{(a_{\frac{p}{2}})} + \frac{p\eta}{2}) \right\} + \ldots\,, \end{aligned} \tag{3.55}$$

where the ellipsis denotes the terms in (3.54) that are independent of Bethe roots. If one works instead with the $T-Q$ relations (3.43), one obtains the same results (3.54), (3.55), except with sums over the b roots.

We have verified the $T-Q$ equations numerically, for values of p and N up to 6 and for generic values of the boundary parameters, along the lines [28]. These results are consistent with the conjecture

$$M_a = \lfloor \frac{N-1}{2} \rfloor + 2p + 1 \,, \qquad M_b = \lfloor \frac{N-1}{2} \rfloor + p \,, \tag{3.56}$$

which agrees with the relation (3.44). These numerical results also indicate that our Bethe Ansatz solution is complete: for each value of N, we find sets of Bethe roots corresponding to each of the 2^N eigenvalues of the transfer matrix. As already remarked, this numerical work provides support for the Ansatz (3.38), (3.39).

3.2 The XX chain ($p = 1$)

The case $p = 1$ corresponds to bulk anisotropy value $\eta = i\pi/2$, for which the bulk Hamiltonian (2.2) reduces to

$$\mathcal{H}_0 = \frac{1}{2} \sum_{n=1}^{N-1} \left(\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y \right) \,, \tag{3.57}$$

which is known as the XX chain. The open XX chain with nondiagonal boundary terms was studied earlier in [25], [54]–[56].

The functional equation for the case $p = 1$ is given by

$$t(u)\; t(u+\eta) - \delta(u) - \delta(u+\eta) = f(u) \,, \tag{3.58}$$

We find that a suitable matrix $M(u)$ is given by

$$\mathcal{M}(u) = \begin{pmatrix} \Lambda(u) & -m_1(u) \\ -n_1(u) & \Lambda(u+\eta) \end{pmatrix} \,, \tag{3.59}$$

where

$$m_1(u) = \frac{1}{h_1(-u)} \Big[h_0(u)\ \delta_1(u+\eta) + h_0(-u-\eta)\ z_1^-(u)\Big] \,, \qquad (3.60)$$

$$n_1(u) = \frac{1}{h_1(u)} \Big[h_0(-u)\ \delta_1(u+\eta) + h_0(u+\eta)\ z_1^+(u)\Big] \,. \qquad (3.61)$$

Indeed, one can verify that the condition $\det \mathcal{M}(u) = 0$ reproduces the functional equation (3.58). Note that

$$n_1(u) = m_1(-u) \,. \qquad (3.62)$$

The corresponding null eigenvector $v(u) = (v_1(u)\,, v_2(u))$ satisfies $\mathcal{M}(u)\ v(u) = 0$, i.e.,

$$\Lambda(u)\ v_1(u) = m_1(u)\ v_2(u) \,, \qquad (3.63)$$

$$\Lambda(u)\ v_2(u-\eta) = n_1(u-\eta)\ v_1(u-\eta) \,. \qquad (3.64)$$

The crossing symmetry $\Lambda(-u-\eta) = \Lambda(u)$ and (3.62) suggest

$$v_2(u) = v_1(-u) \,. \qquad (3.65)$$

That is, only one component is independent, say, $v_1(u)$. Substituting the explicit expression (3.60) into the first equation (3.63), we obtain

$$\Lambda(u)\ v_1(u) = \frac{1}{h_1(-u)} \Big[h_0(u)\ \delta_1(u+\eta) + h_0(-u-\eta)\ z_1^-(u)\Big]\, v_1(-u) \,. \qquad (3.66)$$

Similarly to the $p > 1$ case, we make the Ansatz

$$v_1(u) = a_1(u) + b_1(u)\ Y(u) \,, \qquad (3.67)$$

where

$$a_1(u) = A \prod_{k=1}^{2M_a} \sinh(u - u_k^{(a_1)}) \,, \qquad b_1(u) = \prod_{k=1}^{2M_b} \sinh(u - u_k^{(b_1)}) \,. \qquad (3.68)$$

Substituting this Ansatz, together with the expression for $z_1^-(u)$ (3.17), into (3.66), we obtain the desired generalized $T-Q$ equations:

$$\begin{aligned}\Lambda(u)\ a_1(u)\ h_1(-u) &= \left[h_0(u)\ \delta_1(u+\eta) + \frac{1}{2}h_0(-u-\eta)\ f_1(u)\right] a_1(-u) \\ &- \frac{1}{2}h_0(-u-\eta)\ g_1(u)\ Y(u)^2\ b_1(-u)\,, \qquad (3.69) \\ \Lambda(u)\ b_1(u)\ h_1(-u) &= \left[h_0(u)\ \delta_1(u+\eta) + \frac{1}{2}h_0(-u-\eta)\ f_1(u)\right] b_1(-u) \\ &- \frac{1}{2}h_0(-u-\eta)\ g_1(u)\ a_1(-u)\,. \qquad (3.70)\end{aligned}$$

From the asymptotic behavior we obtain the relation

$$M_a = M_b + 2\,. \qquad (3.71)$$

The corresponding Bethe Ansatz equations are

$$\frac{h_0(-u_l^{(a_1)}-\eta)}{h_0(u_l^{(a_1)})} = -\frac{2\delta_1(u_l^{(a_1)}+\eta)\ a_1(-u_l^{(a_1)})}{f_1(u_l^{(a_1)})\ a_1(-u_l^{(a_1)}) - g_1(u_l^{(a_1)})\ Y(u_l^{(a_1)})^2\ b_1(-u_l^{(a_1)})}\,, \qquad (3.72)$$

$$\frac{h_0(-u_l^{(b_1)}-\eta)}{h_0(u_l^{(b_1)})} = -\frac{2\delta_1(u_l^{(b_1)}+\eta)\ b_1(-u_l^{(b_1)})}{f_1(u_l^{(b_1)})\ b_1(-u_l^{(b_1)}) - g_1(u_l^{(b_1)})\ a_1(-u_l^{(b_1)})}\,, \qquad (3.73)$$

and, e.g.,

$$f_1(\alpha_-)\ b_1(-\alpha_-) = g_1(\alpha_-)\ a_1(-\alpha_-)\,. \qquad (3.74)$$

There are no additional relations arising from analyticity at $u = -\frac{\eta}{2}$ analogous to (3.47), (3.50) due to the identity $f_1(-\frac{\eta}{2}) = 2\delta_1(\frac{\eta}{2})$.

The energy eigenvalues of the Hamiltonian (2.1) follow from (2.9), (2.10) and the first $T-Q$ relation (3.69),

$$\begin{aligned}E &= d_1\Lambda''(0) = d_1 d_0\left[-2\frac{a_1'(0)}{a_1(0)} + \frac{h_1'(0)}{h_1(0)}\right] \\ &= i\sum_{l=1}^{2M_a}\coth u_l^{(a_1)} + \frac{i}{2}\left(\coth\alpha_- + \tanh\beta_- + \coth\alpha_+ + \tanh\beta_+\right)\,. \qquad (3.75)\end{aligned}$$

Working instead with the second $T-Q$ relation (3.70) gives the same result (3.75) except with sums over b roots.

We have verified that the above $T-Q$ equations are well-satisfied numerically, for values of N up to 8 and for generic values of the boundary parameters, along the lines [28]. These results are consistent with the conjecture

$$M_a = \lfloor \frac{N-1}{2} \rfloor + 3 \,, \qquad M_b = \lfloor \frac{N-1}{2} \rfloor + 1 \,, \tag{3.76}$$

which agrees with the relation (3.71), and in fact also with (3.56). These results also indicate that our Bethe Ansatz solution is complete.

We have found a Bethe-Ansatz-type solution of the open spin-1/2 integrable XXZ quantum spin chain with general integrable boundary terms at roots of unity. All six boundary parameters are arbitrary. In particular, the boundary parameters need *not* satisfy the constraint (2.3) that arose in previous work [24], [27]-[29]. Moreover, in contrast to that earlier solution, our new solution appears to give the complete set of 2^N eigenvalues in a straightforward manner. This solution is essentially the same for both even and odd values of p, the main difference being that, in the former case, one of the Q functions is crossing invariant.

Part of the price paid for this success is that there are multiple Q functions $\{a_j(u)\,, b_j(u)\}$ and corresponding multiple sets of Bethe roots $\{u_l^{(a_j)}\,, u_l^{(b_j)}\}$. However, we have already demonstrated the feasibility of performing thermodynamic $(N \to \infty)$ computations with two such sets of Bethe roots [53]. Hence, we expect that this multiplicity of sets of Bethe roots will not cause significant computational difficulty. A further complication is the appearance of normalization constants $\{A_j\,, B_j\}$ and their corresponding Bethe-Ansatz-type equations.

Another part of the price paid for this success is that the bulk anisotropy parameter is restricted to the values $i\pi/(p+1)$. However, we expect that it should be possible to further generalize our solution to the case $\eta = i\pi p'/(p+1)$, where p' is also an integer. Indeed, we expect that functional relations of order $p+1$ with the same structure (e.g., (2.15)) will continue to hold for that case, except with a different function $f(u)$ that will now depend also on p'. Hence, to the extent that a number can be approximated by a rational number, this approach should in principle solve the problem for general imaginary values of η. Unfortunately, this approach does not seem to be suitable for directly addressing the problem of real values of η, for which case the transfer matrix presumably does not obey functional relations of finite order. Nevertheless, as in the case of the sinh-Gordon and sine-Gordon models, it may perhaps be possible to obtain results for real values of η from those of imaginary values of η by some sort of analytic continuation.

Although we have considered here the case of generic values of the boundary parameters for which the quantity $\Delta(u)$ is not a perfect square, we find numerical evidence that our solution remains valid when $\Delta(u)$ becomes a perfect square. Presumably, for such special cases, the Q functions $\{a_j(u)\,, b_j(u)\}$ are not independent. It may be interesting to determine the precise relationship between these Q functions and those appearing in the previously found solutions [24], [27]-[29], [51, 52].

We have also considered the case $\eta = i\pi p/(p+1)$, with p a positive integer, which corresponds to the "reflectionless points" of the sine-Gordon model. Numerical experiments suggest that for p odd, the transfer matrix obeys the same functional relations (with the same function $f(u)$ (2.23),(2.24)) as for the case where $\eta = i\pi/(p+1)$; hence, the same solution also holds for this case. However, for p even, the function $f(u)$ must be slightly modified. The resulting expression is given in Appendix 2.

We remark that the set of off-diagonal elements (3.28) of the matrix $\mathcal{M}(u)$ is not unique. Indeed, we have found other sets of matrix elements which also give $\det \mathcal{M}(u) = 0$. Among all the sets which we found, the particular set presented here has several advantages: (i) it works for both even and odd values of p; (ii) the corresponding $T - Q$ relations and Bethe Ansatz equations are relatively simple; (iii) the corresponding values of M_a and M_b are minimized. Nevertheless, it may be worthwhile to continue looking for alternative sets of off-diagonal matrix elements, which may further reduce the values of M_a and M_b, or which may have other nice properties.

A key step in our analysis is the Ansatz (3.38), (3.39), which allows us to express the non-analytic quantities $\{v_j(u)\}$ in terms of analytic ones $\{a_j(u)\,, b_j(u)\}$. We have numerical evidence that this Ansatz is valid. However, it is not clear whether this Ansatz is the most "economical": there may be alternative Ansätze which introduce fewer Q functions. For example, there may be some fixed relation between $a_j(u)$ and $b_j(u)$.

The structure of our generalized $T - Q$ equations bears some resemblance to that of the conventional TBA equations of the XXZ chain [56]. Presumably, this common structure has its origin in the fusion rules and root of unity properties of the underlying $U_q(su_2)$ algebra.

Having in hand an exact solution of a model with so many free boundary parameters, one can hope to be able to analyze a plethora of interesting boundary behavior.

Finally, we note that it should be possible to generalize the approach presented here to open integrable anisotropic spin chains constructed from R and K matrices (both trigonometric and elliptic) corresponding to higher-dimensional representations and/or higher-rank algebras.

Chapter 4: Boundary Energy of The Open XXZ Chain From New Exact Solutions

Bethe Ansatz solutions with up to two free boundary parameters have been proposed in [51, 52]. Completeness of these new solutions is straightforward, in contrast to the case (2.3) [28]. A noteworthy feature of the solution [52] is the appearance of a *generalized* $T-Q$ relation of the form

$$\begin{aligned} t(u)\ Q_1(u) &= Q_2(u') + Q_2(u'')\,, \\ t(u)\ Q_2(u) &= Q_1(u') + Q_1(u'')\,, \end{aligned} \tag{4.1}$$

involving two Q-operators, instead of the usual one [35]. However, unlike the case (2.3), these new solutions hold only at roots of unity, i.e., bulk anisotropy values (2.70) for all positive integer values of p .

The aim of this chapter is to use the new solutions [51, 52] to investigate the ground state in the thermodynamic ($N \to \infty$) limit. For definiteness, we focus on two particular cases:

Case I: The bulk anisotropy parameter has values (2.70) with p *even*;

the boundary parameters $\beta_\pm$ are arbitrary, and $\alpha_\pm = \eta$, $\theta_\pm = 0$ [51] (4.2)

Case II: The bulk anisotropy parameter has values (2.70) with p *odd*;

the boundary parameters $\alpha_\pm$ are arbitrary, and $\beta_\pm = \theta_\pm = 0$ [52] (4.3)

We also henceforth restrict to even values of N. For each of these cases, we determine the density of Bethe roots describing the ground state in the thermodynamic limit, for suitable values of the boundary parameters; and we compute the corresponding boundary (surface) energies. [12] We find that the results coincide with the boundary energy computed in [42] for the case (2.3), namely, [13]

$$\begin{aligned} E^{\pm}_{boundary} &= -\frac{\sin\mu}{2\mu}\int_{-\infty}^{\infty} d\omega\ \frac{1}{2\cosh(\omega/2)}\Big\{\frac{\sinh((\nu-2)\omega/4)}{2\sinh(\nu\omega/4)} - \frac{1}{2} \\ &+ \operatorname{sgn}(2a_{\pm}-1)\frac{\sinh((\nu-|2a_{\pm}-1|)\omega/2)}{\sinh(\nu\omega/2)} + \frac{\sinh(\omega/2)\cos(b_{\pm}\omega)}{\sinh(\nu\omega/2)}\Big\} \\ &+ \frac{1}{2}\sin\mu\cot(\mu a_{\pm}) - \frac{1}{4}\cos\mu\,, \end{aligned} \tag{4.4}$$

where

$$\mu = -i\eta = \frac{\pi}{p+1}\,, \quad \nu = \frac{\pi}{\mu} = p+1\,, \quad \alpha_{\pm} = i\mu a_{\pm}\,, \quad \beta_{\pm} = \mu b_{\pm}\,, \tag{4.5}$$

and $\operatorname{sgn}(n) = \frac{n}{|n|}$ for $n \neq 0$.

4.1 Case I: p even

For Case I (4.2), the Hamiltonian (2.1) becomes

$$\mathcal{H} = \mathcal{H}_0 + \frac{1}{2}\left(\cosh\eta\tanh\beta_{-}\sigma_1^z + \operatorname{sech}\beta_{-}\sigma_1^x - \cosh\eta\tanh\beta_{+}\sigma_N^z + \operatorname{sech}\beta_{+}\sigma_N^x\right) \tag{4.6}$$

which is Hermitian for $\beta_{\pm}$ real. The eigenvalues $\Lambda(u)$ of the transfer matrix (1.11) are given by [51]

$$\Lambda(u) = h(u)\frac{Q(u+p\eta)}{Q(u)} + h(-u-\eta)\frac{Q(u-p\eta)}{Q(u)}\,, \tag{4.7}$$

where [14]

$$\begin{aligned} h(u) &= 4\sinh^{2N+1}(u+\eta)\frac{\sinh(2u+2\eta)}{\sinh(2u+\eta)}\sinh(u-\eta) \\ &\times \left(\cosh u + i\sinh\beta_{-}\right)\left(\cosh u - i\sinh\beta_{+}\right)\,, \end{aligned} \tag{4.8}$$

[12] For the case of diagonal boundary terms, the boundary energy was first computed numerically in [15], and then analytically in [57].

[13] Here we correct the misprint in Eq. (2.29) in [42], as already noted in [43].

[14] We find that the function $h(u)$ given by (2.81), to which we now refer as $h_{old}(u)$, leads to $p-1$ "Bethe roots" which actually are common to all the eigenvalues, and which therefore should be incorporated into a new $h(u)$. In this way, we arrive at the expression (4.8), which is equal to $h_{old}(u)\frac{\sinh(u+\eta)}{\sinh(u-\eta)}$; and at the M value in (4.9), which is equal to $M_{old}-(p-1)$, where M_{old} is given by (2.82).

and

$$Q(u) = \prod_{j=1}^{M} \sinh\left(\frac{1}{2}(u-u_j)\right) \sinh\left(\frac{1}{2}(u+u_j+\eta)\right) \,, \qquad M = N + p \,. \tag{4.9}$$

The zeros u_j of $Q(u)$ satisfy the Bethe Ansatz equations

$$\frac{h(u_j)}{h(-u_j-\eta)} = -\frac{Q(u_j - p\eta)}{Q(u_j + p\eta)} \,, \qquad j = 1 \,, \ldots \,, M \,. \tag{4.10}$$

More explicitly, in terms of the "shifted" Bethe roots $\tilde{u}_j \equiv u_j + \frac{\eta}{2}$,

$$\begin{aligned} &\left(\frac{\sinh(\tilde{u}_j + \frac{\eta}{2})}{\sinh(\tilde{u}_j - \frac{\eta}{2})}\right)^{2N+1} \frac{\sinh(2\tilde{u}_j + \eta)}{\sinh(2\tilde{u}_j - \eta)} \frac{\sinh(\tilde{u}_j - \frac{3\eta}{2})}{\sinh(\tilde{u}_j + \frac{3\eta}{2})} \\ &\quad \times \left(\frac{\cosh(\tilde{u}_j - \frac{\eta}{2}) + i \sinh \beta_-}{\cosh(\tilde{u}_j + \frac{\eta}{2}) + i \sinh \beta_-}\right) \left(\frac{\cosh(\tilde{u}_j - \frac{\eta}{2}) - i \sinh \beta_+}{\cosh(\tilde{u}_j + \frac{\eta}{2}) - i \sinh \beta_+}\right) \\ &\quad = -\prod_{k=1}^{M} \frac{\cosh(\frac{1}{2}(\tilde{u}_j - \tilde{u}_k + \eta))}{\cosh(\frac{1}{2}(\tilde{u}_j - \tilde{u}_k - \eta))} \frac{\cosh(\frac{1}{2}(\tilde{u}_j + \tilde{u}_k + \eta))}{\cosh(\frac{1}{2}(\tilde{u}_j + \tilde{u}_k - \eta))} \,, \quad j = 1 \,, \cdots \,, M \end{aligned} \tag{4.11}$$

The energy eigenvalues are given by (2.6)

$$\begin{aligned} E &= c_1 \Lambda'(0) + c_2 \\ &= c_1 h(0) \frac{Q(p\eta)}{Q(0)} \left[\frac{h'(0)}{h(0)} + \frac{Q'(p\eta)}{Q(p\eta)} - \frac{Q'(0)}{Q(0)}\right] + c_2 \,. \end{aligned} \tag{4.12}$$

Using the fact

$$\Lambda(0) = h(0) \frac{Q(p\eta)}{Q(0)} = c_0 \,, \tag{4.13}$$

where the second equality follows from (2.8), we arrive at the result

$$E = \frac{1}{2} \sinh^2 \eta \sum_{j=1}^{M} \frac{1}{\sinh(\tilde{u}_j - \frac{\eta}{2}) \sinh(\tilde{u}_j + \frac{\eta}{2})} + \frac{1}{2}(N-1) \cosh \eta \,. \tag{4.14}$$

Numerical investigation of the ground state for small values of N and p (along the lines of [28]) suggests making a further shift of the Bethe roots,

$$\tilde{\tilde{u}}_j \equiv \tilde{u}_j - \frac{i\pi}{2} = u_j + \frac{\eta}{2} - \frac{i\pi}{2} \,, \tag{4.15}$$

in terms of which the Bethe Ansatz Eqs. (4.11) become

$$\left(\frac{\cosh(\tilde{\tilde{u}}_j + \frac{\eta}{2})}{\cosh(\tilde{\tilde{u}}_j - \frac{\eta}{2})}\right)^{2N+2} \frac{\sinh(\tilde{\tilde{u}}_j + \frac{\eta}{2})}{\sinh(\tilde{\tilde{u}}_j - \frac{\eta}{2})} \frac{\cosh(\tilde{\tilde{u}}_j - \frac{3\eta}{2})}{\cosh(\tilde{\tilde{u}}_j + \frac{3\eta}{2})}$$
$$\times \frac{\sinh(\frac{1}{2}(\tilde{\tilde{u}}_j + \beta_- - \frac{\eta}{2}))\cosh(\frac{1}{2}(\tilde{\tilde{u}}_j - \beta_- - \frac{\eta}{2}))}{\sinh(\frac{1}{2}(\tilde{\tilde{u}}_j + \beta_- + \frac{\eta}{2}))\cosh(\frac{1}{2}(\tilde{\tilde{u}}_j - \beta_- + \frac{\eta}{2}))}$$
$$\times \frac{\sinh(\frac{1}{2}(\tilde{\tilde{u}}_j - \beta_+ - \frac{\eta}{2}))\cosh(\frac{1}{2}(\tilde{\tilde{u}}_j + \beta_+ - \frac{\eta}{2}))}{\sinh(\frac{1}{2}(\tilde{\tilde{u}}_j - \beta_+ + \frac{\eta}{2}))\cosh(\frac{1}{2}(\tilde{\tilde{u}}_j + \beta_+ + \frac{\eta}{2}))}$$
$$= -\prod_{k=1}^{M} \frac{\cosh(\frac{1}{2}(\tilde{\tilde{u}}_j - \tilde{\tilde{u}}_k + \eta))}{\cosh(\frac{1}{2}(\tilde{\tilde{u}}_j - \tilde{\tilde{u}}_k - \eta))} \frac{\sinh(\frac{1}{2}(\tilde{\tilde{u}}_j + \tilde{\tilde{u}}_k + \eta))}{\sinh(\frac{1}{2}(\tilde{\tilde{u}}_j + \tilde{\tilde{u}}_k - \eta))} \,, \quad j = 1\,, \cdots, M \tag{4.16}$$

Moreover, we find that for suitable values of the boundary parameters $\beta_\pm$ (which we discuss after Eq. (4.38) below), the $N+p$ Bethe roots $\{\tilde{\tilde{u}}_1\,, \ldots\,, \tilde{\tilde{u}}_{N+p}\}$ for the ground state have the approximate form [15]

$$\left\{ \begin{array}{ccc} v_j \pm \frac{i\pi}{2} & : & j = 1\,,2\,,\ldots\,,\frac{N}{2} \\ v_j^{(1)} + i\pi\,, \quad v_j^{(2)} & : & j = 1\,,2\,,\ldots\,,\frac{p}{2} \end{array} \right. \,, \tag{4.17}$$

where $\{v_j\,, v_j^{(a)}\}$ are all *real* and positive. That is, the ground state is described by $\frac{N}{2}$ "strings" of length 2, and $\frac{p}{2}$ pairs of strings of length 1.

We make the "string hypothesis" that (4.17) is exactly true in the thermodynamic limit ($N \to \infty$ with p fixed). The number of strings of length 2 therefore becomes infinite (there is a "sea" of such 2-strings); and the distribution of their centers $\{v_j\}$ is described by a density function, which can be computed from the counting function. To this end, we form the product of the Bethe Ansatz Eqs. (4.16) for the sea roots $v_j \pm \frac{i\pi}{2}$. The result is given by

$$e_1(\lambda_j)^{4N+4} g_1(\lambda_j)^2 \left[e_3(\lambda_j)^2 g_{1+i2b_-}(\lambda_j) g_{1-i2b_-}(\lambda_j) g_{1+i2b_+}(\lambda_j) g_{1-i2b_+}(\lambda_j)\right]^{-1} \tag{4.18}$$
$$= \left[\prod_{k=1}^{N/2} e_2(\lambda_j - \lambda_k) e_2(\lambda_j + \lambda_k)\right]^2 \prod_{a=1}^{2} \prod_{k=1}^{p/2} \left[g_2(\lambda_j - \lambda_k^{(a)}) g_2(\lambda_j + \lambda_k^{(a)})\right] \,,$$
$$j = 1\,, \ldots\,, \frac{N}{2}\,,$$

[15]Due to the periodicity and crossing properties $Q(u + 2i\pi) = Q(-u - \eta) = Q(u)$, the zeros u_j are defined up to $u_j \mapsto u_j + 2i\pi$ and $u_j \mapsto -u_j - \eta$, which corresponds to $\tilde{\tilde{u}}_j \mapsto \tilde{\tilde{u}}_j + 2i\pi$ and $\tilde{\tilde{u}}_j \mapsto -\tilde{\tilde{u}}_j - i\pi$, respectively. We use these symmetries to restrict the roots to the fundamental region $\Re e\ \tilde{\tilde{u}}_j \ge 0$ and $-\pi < \Im m\ \tilde{\tilde{u}}_j \le \pi$.

where we have used the notation (4.5), as well as

$$v_j = \mu\lambda_j \,, \qquad v_j^{(a)} = \mu\lambda_j^{(a)} \,, \tag{4.19}$$

and (see [42] and references therein)

$$e_n(\lambda) = \frac{\sinh\left(\mu(\lambda + \frac{in}{2})\right)}{\sinh\left(\mu(\lambda - \frac{in}{2})\right)} \,, \qquad g_n(\lambda) = e_n(\lambda \pm \frac{i\pi}{2\mu}) = \frac{\cosh\left(\mu(\lambda + \frac{in}{2})\right)}{\cosh\left(\mu(\lambda - \frac{in}{2})\right)} \,. \tag{4.20}$$

Taking the logarithm of (4.18), we obtain the ground-state counting function

$$\begin{aligned} \mathsf{h}(\lambda) = \frac{1}{4\pi}\Big\{ & (4N+4) q_1(\lambda) + 2 r_1(\lambda) - 2 q_3(\lambda) \\ & - r_{1+i2b_-}(\lambda) - r_{1-i2b_-}(\lambda) - r_{1+i2b_+}(\lambda) - r_{1-i2b_+}(\lambda) \\ & -2\sum_{k=1}^{N/2}\left[q_2(\lambda-\lambda_k) + q_2(\lambda+\lambda_k)\right] - \sum_{a=1}^{2}\sum_{k=1}^{p/2}\left[r_2(\lambda-\lambda_k^{(a)}) + r_2(\lambda+\lambda_k^{(a)})\right]\Big\} \end{aligned} \tag{4.21}$$

where $q_n(\lambda)$ and $r_n(\lambda)$ are odd functions defined by

$$\begin{aligned} q_n(\lambda) &= \pi + i \ln e_n(\lambda) = 2\tan^{-1}\left(\cot(n\mu/2)\tanh(\mu\lambda)\right) \,, \\ r_n(\lambda) &= i \ln g_n(\lambda) \,. \end{aligned} \tag{4.22}$$

Noting that

$$\sum_{k=1}^{N/2}\left[q_2(\lambda-\lambda_k) + q_2(\lambda+\lambda_k)\right] = \sum_{k=-N/2}^{N/2} q_2(\lambda-\lambda_k) - q_2(\lambda) \,, \tag{4.23}$$

where $\lambda_{-k} \equiv -\lambda_k$, and letting N become large, we obtain a linear integral equation for the ground-state root density $\rho(\lambda)$,

$$\rho(\lambda) = \frac{1}{N}\frac{d\mathsf{h}}{d\lambda} = 2a_1(\lambda) - \int_{-\infty}^{\infty} d\lambda' \; a_2(\lambda-\lambda') \; \rho(\lambda') \tag{4.24}$$

$$\begin{aligned} &+ \frac{1}{2N}\Big\{4a_1(\lambda) + 2b_1(\lambda) - 2a_3(\lambda) + 2a_2(\lambda) - b_{1+2ib_-}(\lambda) - b_{1-2ib_-}(\lambda) \\ &- b_{1+2ib_+}(\lambda) - b_{1-2ib_+}(\lambda) - \sum_{a=1}^{2}\sum_{k=1}^{p/2}\left[b_2(\lambda-\lambda_k^{(a)}) + b_2(\lambda+\lambda_k^{(a)})\right]\Big\} \,, \end{aligned} \tag{4.25}$$

where we have ignored corrections of higher order in $1/N$ when passing from a sum to an integral, and we have introduced the notations

$$\begin{aligned} a_n(\lambda) &= \frac{1}{2\pi}\frac{d}{d\lambda}q_n(\lambda) = \frac{\mu}{\pi}\frac{\sin(n\mu)}{\cosh(2\mu\lambda)-\cos(n\mu)}\,, \\ b_n(\lambda) &= \frac{1}{2\pi}\frac{d}{d\lambda}r_n(\lambda) = -\frac{\mu}{\pi}\frac{\sin(n\mu)}{\cosh(2\mu\lambda)+\cos(n\mu)}\,. \end{aligned} \tag{4.26}$$

Using Fourier transforms, we obtain [16]

$$\rho(\lambda) = 2s(\lambda) + \frac{1}{N}R(\lambda)\,, \tag{4.27}$$

where

$$s(\lambda) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\ e^{-i\omega\lambda}\frac{1}{2\cosh(\omega/2)} = \frac{1}{2\cosh(\pi\lambda)}\,, \tag{4.28}$$

and

$$\begin{aligned} \hat{R}(\omega) &= \frac{1}{2\left(1+\hat{a}_2(\omega)\right)}\Big\{4\hat{a}_1(\omega) + 2\hat{b}_1(\omega) - 2\hat{a}_3(\omega) + 2\hat{a}_2(\omega) - \hat{b}_{1+2ib_-}(\omega) \\ &- \hat{b}_{1-2ib_-}(\omega) - \hat{b}_{1+2ib_+}(\omega) - \hat{b}_{1-2ib_+}(\omega) - 2\sum_{a=1}^{2}\sum_{k=1}^{p/2}\cos(\omega\lambda_k^{(a)})\ \hat{b}_2(\omega)\Big\} \end{aligned} \tag{4.29}$$

with

$$\hat{a}_n(\omega) = \mathrm{sgn}(n)\frac{\sinh\left((\nu-|n|)\omega/2\right)}{\sinh\left(\nu\omega/2\right)}\,, \qquad 0 \le |n| < 2\nu\,, \tag{4.30}$$

$$\hat{b}_n(\omega) = -\frac{\sinh\left(n\omega/2\right)}{\sinh\left(\nu\omega/2\right)}\,, \qquad 0 < \Re e\ n < \nu\,. \tag{4.31}$$

Turning now to the expression (4.14) for the energy, and invoking again the string hypothesis (4.17), we see that

$$E = -\frac{1}{2}\sinh^2\eta\sum_{j=1}^{M}\frac{1}{\cosh(\tilde{\tilde{u}}_j-\frac{\eta}{2})\cosh(\tilde{\tilde{u}}_j+\frac{\eta}{2})} + \frac{1}{2}(N-1)\cosh\eta$$

[16] Our conventions are

$$\hat{f}(\omega) \equiv \int_{-\infty}^{\infty} e^{i\omega\lambda}\ f(\lambda)\ d\lambda\,, \qquad f(\lambda) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\omega\lambda}\ \hat{f}(\omega)\ d\omega\,.$$

$$
\begin{aligned}
&= -\frac{1}{2}\sinh^2\eta\Big\{-2\sum_{j=1}^{N/2}\frac{1}{\sinh(v_j-\frac{\eta}{2})\sinh(v_j+\frac{\eta}{2})} \\
&+ \sum_{a=1}^{2}\sum_{j=1}^{p/2}\frac{1}{\cosh(v_j^{(a)}-\frac{\eta}{2})\cosh(v_j^{(a)}+\frac{\eta}{2})}\Big\}+\frac{1}{2}(N-1)\cosh\eta \\
&= -\frac{2\pi\sin\mu}{\mu}\Big\{\sum_{j=1}^{N/2}a_1(\lambda_j)+\frac{1}{2}\sum_{a=1}^{2}\sum_{j=1}^{p/2}b_1(\lambda_j^{(a)})\Big\}+\frac{1}{2}(N-1)\cos\mu\,. \qquad (4.32)
\end{aligned}
$$

Repeating the maneuver (4.23) in the summation over the centers of the sea roots, and letting N become large, we obtain

$$
\begin{aligned}
E &= -\frac{\pi\sin\mu}{\mu}\Big\{\sum_{j=-N/2}^{N/2}a_1(\lambda_j)-a_1(0)+\sum_{a=1}^{2}\sum_{j=1}^{p/2}b_1(\lambda_j^{(a)})\Big\}+\frac{1}{2}(N-1)\cos\mu \qquad (4.33)\\
&= -\frac{\pi\sin\mu}{\mu}\Big\{N\int_{-\infty}^{\infty}d\lambda\ a_1(\lambda)\ \rho(\lambda)-a_1(0)+\sum_{a=1}^{2}\sum_{j=1}^{p/2}b_1(\lambda_j^{(a)})\Big\}+\frac{1}{2}(N-1)\cos\mu\,,
\end{aligned}
$$

where again we ignore corrections that are higher order in $1/N$. Substituting the result (4.27) for the root density, we obtain

$$
E = E_{bulk} + E_{boundary}\,, \qquad (4.34)
$$

where the bulk (order N) energy is given by

$$
\begin{aligned}
E_{bulk} &= -\frac{2N\pi\sin\mu}{\mu}\int_{-\infty}^{\infty}d\lambda\ a_1(\lambda)\ s(\lambda)+\frac{1}{2}N\cos\mu \\
&= -N\sin^2\mu\int_{-\infty}^{\infty}d\lambda\ \frac{1}{[\cosh(2\mu\lambda)-\cos\mu]\cosh(\pi\lambda)}+\frac{1}{2}N\cos\mu\,, \qquad (4.35)
\end{aligned}
$$

which agrees with the well-known result [13]. Moreover, the boundary (order 1) energy is given by

$$
E_{boundary} = -\frac{\pi\sin\mu}{\mu}\Big\{I+\sum_{a=1}^{2}\sum_{j=1}^{p/2}b_1(\lambda_j^{(a)})\Big\}-\frac{1}{2}\cos\mu\,, \qquad (4.36)
$$

where I is the integral

$$
\begin{aligned}
I &= \int_{-\infty}^{\infty}d\lambda\ a_1(\lambda)\,[R(\lambda)-\delta(\lambda)] = \frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\ \hat{a}_1(\omega)\left[\hat{R}(\omega)-1\right] \\
&= -\sum_{a=1}^{2}\sum_{j=1}^{p/2}b_1(\lambda_j^{(a)})+\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\ \hat{s}(\omega)\Big\{2\hat{a}_1(\omega)+\hat{b}_1(\omega)-\hat{a}_3(\omega)-1 \\
&\quad -\frac{1}{2}\left[\hat{b}_{1+2ib_-}(\omega)+\hat{b}_{1-2ib_-}(\omega)+\hat{b}_{1+2ib_+}(\omega)+\hat{b}_{1-2ib_+}(\omega)\right]\Big\}\,, \qquad (4.37)
\end{aligned}
$$

where we have used the fact $\hat{s}(\omega)\hat{b}_2(\omega) = \hat{b}_1(\omega)$. Remarkably, the $\lambda_j^{(a)}$-dependent contribution in (4.36) is exactly canceled by an opposite contribution from the integral I (4.37). Writing the boundary energy as the sum of contributions from the left and right boundaries, $E_{boundary} = E^-_{boundary} + E^+_{boundary}$, we conclude that the energy contribution from each boundary is given by

$$\begin{aligned} E^{\pm}_{boundary} &= -\frac{\sin\mu}{2\mu}\int_{-\infty}^{\infty} d\omega\, \frac{1}{2\cosh(\omega/2)}\Big\{\frac{\sinh((\nu-2)\omega/4)}{2\sinh(\nu\omega/4)} - \frac{1}{2} \\ &+ \frac{\sinh(\omega/2)\cosh((\nu-2)\omega/2)}{\sinh(\nu\omega/2)} + \frac{\sinh(\omega/2)\cos(b_{\pm}\omega)}{\sinh(\nu\omega/2)}\Big\} - \frac{1}{4}\cos\mu\,. \end{aligned} \tag{4.38}$$

One can verify that this result coincides with the result (4.4) with $a_{\pm} = 1$. As shown in Appendix 3, the integrals in (4.35) and (4.38) (with p even) can be evaluated analytically.

We have derived the result (4.38) for the boundary energy under the assumption that the Bethe roots for the ground state have the form (4.17), which is true only for suitable values of the boundary parameters $\beta_{\pm}$. For example, the shaded region in Fig. 4.1 denotes the region of parameter space for which the ground-state Bethe roots have the form (4.17) for $p = 4$ and $N = 2$. For parameter values outside the shaded region, one or more of the Bethe roots has an imaginary part which is *not* a multiple of $\pi/2$ and which evidently depends on the parameter values (but in a manner which we have not yet explicitly determined). As p increases, the figure is similar, except that the shaded region moves further away from the origin.

A qualitative explanation of these features can be deduced from a short heuristic argument. Indeed, let us rewrite the Hamiltonian (4.6) as

$$\mathcal{H} = \mathcal{H}_0 + h_1^z\sigma_1^z + h_1^x\sigma_1^x + h_N^z\sigma_N^z + h_N^x\sigma_N^x\,, \tag{4.39}$$

where the boundary magnetic fields are given by

$$h_1^z = \frac{1}{2}\cosh\eta\tanh\beta_-\,, \quad h_1^x = \frac{1}{2}\operatorname{sech}\beta_-$$

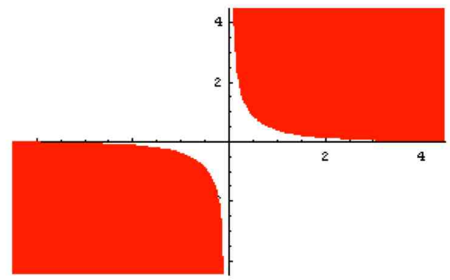

Figure 4.1: Shaded region denotes region of the (β_+ , β_-) plane for which the ground-state Bethe roots have the form (4.17) for $p = 4$ and $N = 2$.

$$h_N^z = -\frac{1}{2} \cosh \eta \tanh \beta_+ , \quad h_N^x = \frac{1}{2} \operatorname{sech} \beta_+ . \tag{4.40}$$

For $\beta_+ \beta_- \gg 0$ (i.e., the shaded regions in Fig. 1), the boundary fields in the x direction are small; moreover, $h_1^z h_N^z < 0$; i.e., the boundary fields in the z direction have antiparallel orientations, which (since N is even) is compatible with a Néel-like (antiferromagnetic) alignment of the spins. (See Fig. 4.2.) Hence, the ground state and corresponding Bethe roots are "simple."

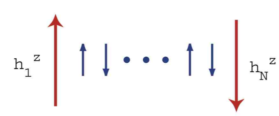

Figure 4.2: Antiparallel boundary fields (big, red) **are** compatible with antiferromagnetic alignment of spins (small, blue)

On the other hand, if $|\beta_\pm|$ are small (the unshaded region near the origin of Fig. 4.1), then the boundary fields in the x direction are large. Also, if $\beta_+ \beta_- < 0$ (the second and fourth quadrants of Fig. 4.1, which are also unshaded), then $h_1^z h_N^z > 0$; i.e., the boundary fields in the z direction are parallel, which can lead to "frustration." (See Fig. 4.3.) For these cases, the ground states and corresponding Bethe roots are "complicated."

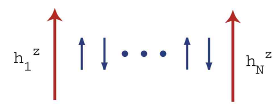

Figure 4.3: Parallel boundary fields (big, red) are **not** compatible with antiferromagnetic alignment of spins (small, blue)

4.2 Case II: p odd

For Case II (4.3), the Hamiltonian (2.1) becomes

$$\mathcal{H} = \mathcal{H}_0 + \frac{1}{2}\sinh\eta\left(\text{cosech}\,\alpha_-\sigma_1^x + \text{cosech}\,\alpha_+\sigma_N^x\right) . \tag{4.41}$$

We restrict $\alpha_\pm$ to be purely imaginary in order for the Hamiltonian to be Hermitian. We use the periodicity $\alpha_\pm \mapsto \alpha_\pm + 2\pi i$ of the transfer matrix to further restrict $\alpha_\pm$ to the fundamental domain $-\pi \le \Im m\ \alpha_\pm < \pi$. The eigenvalues $\Lambda(u)$ of the transfer matrix (1.11) are given by [52] [17]

$$\begin{aligned}\Lambda(u) &= \frac{\delta(u-\eta)}{h^{(2)}(u-\eta)}\frac{Q_2(u-\eta)}{Q_1(u)} + \frac{\delta(u)}{h^{(1)}(u)}\frac{Q_2(u+\eta)}{Q_1(u)}\,,\\ &= h^{(1)}(u-\eta)\frac{Q_1(u-\eta)}{Q_2(u)} + h^{(2)}(u)\frac{Q_1(u+\eta)}{Q_2(u)}\,,\end{aligned} \tag{4.42}$$

where [18]

$$\begin{aligned}h^{(1)}(u) &= \frac{8\sinh^{2N+1}(u+2\eta)\cosh^2(u+\eta)\cosh(u+2\eta)}{\sinh(2u+3\eta)}\,,\\ h^{(2)}(u) &= h^{(1)}(-u-2\eta)\,,\\ \delta(u) &= h^{(1)}(u)h^{(2)}(u)\sinh(u+\eta+\alpha_-)\sinh(u+\eta-\alpha_-)\\ &\times\ \sinh(u+\eta+\alpha_+)\sinh(u+\eta-\alpha_+)\,,\end{aligned} \tag{4.43}$$

[17] The function $Q_2(u)$ here as well as its zeros $\{u_j^{(2)}\}$ are shifted by η with respect to the corresponding quantities in [52], to which we now refer as "old"; i.e., $Q_2(u) = Q_2^{old}(u-\eta)$ and $u_j^{(2)} = u_j^{(2)\ old} - \eta$.

[18] Similarly to Case I, we find that the functions $h^{(1)}(u)$ given in Eqs. (2.125), (2.126) lead to "Bethe roots" which actually are common to all the eigenvalues, and which therefore should be incorporated into a new $h^{(1)}(u)$. In this way, we arrive at the expression for $h^{(1)}(u)$ in (4.43) and the corresponding M_a values in (4.45).

and

$$Q_a(u) = \prod_{j=1}^{M_a} \sinh(u - u_j^{(a)}) \sinh(u + u_j^{(a)} + \eta) \,, \qquad a = 1\,,2\,, \tag{4.44}$$

with

$$M_1 = \frac{1}{2}(N + p + 1)\,, \qquad M_2 = \frac{1}{2}(N + p - 1)\,. \tag{4.45}$$

As remarked earlier in this chapter, the expressions for the eigenvalues (4.42) correspond to generalized $T - Q$ relations (4.1). For generic values of $\alpha_\pm$, we have not managed to reformulate this solution in terms of a single $Q(u)$. The zeros $\{u_j^{(a)}\}$ of $Q_a(u)$ are given by the Bethe Ansatz equations,

$$\begin{aligned} \frac{\delta(u_j^{(1)})\ h^{(2)}(u_j^{(1)} - \eta)}{\delta(u_j^{(1)} - \eta)\ h^{(1)}(u_j^{(1)})} &= -\frac{Q_2(u_j^{(1)} - \eta)}{Q_2(u_j^{(1)} + \eta)}\,, \qquad j = 1\,,2\,,\ldots\,,M_1\,, \\ \frac{h^{(1)}(u_j^{(2)} - \eta)}{h^{(2)}(u_j^{(2)})} &= -\frac{Q_1(u_j^{(2)} + \eta)}{Q_1(u_j^{(2)} - \eta)}\,, \qquad j = 1\,,2\,,\ldots\,,M_2\,. \end{aligned} \tag{4.46}$$

In terms of the "shifted" Bethe roots $\tilde{u}_j^{(a)} \equiv u_j^{(a)} + \frac{\eta}{2}$, the Bethe Ansatz equations are

$$\begin{aligned} &\left(\frac{\sinh(\tilde{u}_j^{(1)} + \frac{\eta}{2})}{\sinh(\tilde{u}_j^{(1)} - \frac{\eta}{2})}\right)^{2N+1} \frac{\cosh(\tilde{u}_j^{(1)} - \frac{\eta}{2})}{\cosh(\tilde{u}_j^{(1)} + \frac{\eta}{2})} \\ &\quad\times \frac{\sinh(\tilde{u}_j^{(1)} + \alpha_- - \frac{\eta}{2})}{\sinh(\tilde{u}_j^{(1)} - \alpha_- + \frac{\eta}{2})} \frac{\sinh(\tilde{u}_j^{(1)} - \alpha_- - \frac{\eta}{2})}{\sinh(\tilde{u}_j^{(1)} + \alpha_- + \frac{\eta}{2})} \frac{\sinh(\tilde{u}_j^{(1)} + \alpha_+ - \frac{\eta}{2})}{\sinh(\tilde{u}_j^{(1)} - \alpha_+ + \frac{\eta}{2})} \frac{\sinh(\tilde{u}_j^{(1)} - \alpha_+ - \frac{\eta}{2})}{\sinh(\tilde{u}_j^{(1)} + \alpha_+ + \frac{\eta}{2})} \\ &\quad = -\prod_{k=1}^{M_2} \frac{\sinh(\tilde{u}_j^{(1)} - \tilde{u}_k^{(2)} + \eta)}{\sinh(\tilde{u}_j^{(1)} - \tilde{u}_k^{(2)} - \eta)} \frac{\sinh(\tilde{u}_j^{(1)} + \tilde{u}_k^{(2)} + \eta)}{\sinh(\tilde{u}_j^{(1)} + \tilde{u}_k^{(2)} - \eta)}\,, \qquad j = 1\,,\cdots\,,M_1\,. \end{aligned} \tag{4.47}$$

and

$$\begin{aligned} &\left(\frac{\sinh(\tilde{u}_j^{(2)} + \frac{\eta}{2})}{\sinh(\tilde{u}_j^{(2)} - \frac{\eta}{2})}\right)^{2N+1} \frac{\cosh(\tilde{u}_j^{(2)} - \frac{\eta}{2})}{\cosh(\tilde{u}_j^{(2)} + \frac{\eta}{2})} \\ &\quad = -\prod_{k=1}^{M_1} \frac{\sinh(\tilde{u}_j^{(2)} - \tilde{u}_k^{(1)} + \eta)}{\sinh(\tilde{u}_j^{(2)} - \tilde{u}_k^{(1)} - \eta)} \frac{\sinh(\tilde{u}_j^{(2)} + \tilde{u}_k^{(1)} + \eta)}{\sinh(\tilde{u}_j^{(2)} + \tilde{u}_k^{(1)} - \eta)}\,, \qquad j = 1\,,\cdots\,,M_2 \end{aligned} \tag{4.48}$$

The energy is given by

$$E = \frac{1}{2}\sinh^2\eta \sum_{a=1}^{2}\sum_{j=1}^{M_a} \frac{1}{\sinh(\tilde{u}_j^{(a)} - \frac{\eta}{2})\sinh(\tilde{u}_j^{(a)} + \frac{\eta}{2})} + \frac{1}{2}(N-1)\cosh\eta\,. \tag{4.49}$$

Indeed, for $p > 1$, we obtain this result by following steps similar to those leading to (4.14). For $p = 1$, we use (2.9) and (2.10) instead of (2.8) and (2.6); nevertheless, the result (4.49) holds also for $p = 1$.

From numerical studies for small values of N and p, and for suitable values of the boundary parameters $\alpha_\pm$ (which we discuss after Eq. (4.66) below), we find that the ground state is described by Bethe roots $\{\tilde{u}_j^{(1)}\}$ and $\{\tilde{u}_j^{(2)}\}$ of the form [19]

$$\left\{ \begin{array}{lcl} v_j^{(1,1)} & : & j = 1\,, 2\,, \ldots\,, \frac{N}{2} \\ v_j^{(1,2)} + \frac{i\pi}{2}\,, & : & j = 1\,, 2\,, \ldots\,, \frac{p+1}{2} \end{array} \right. , \qquad \left\{ \begin{array}{lcl} v_j^{(2,1)} & : & j = 1\,, 2\,, \ldots\,, \frac{N}{2} \\ v_j^{(2,2)} + \frac{i\pi}{2}\,, & : & j = 1\,, 2\,, \ldots\,, \frac{p-1}{2} \end{array} \right. \tag{4.50}$$

respectively, where $\{v_j^{(a,b)}\}$ are all real and positive.

We make the "string hypothesis" that (4.50) remains true in the thermodynamic limit ($N \to \infty$ with p fixed). That is, that the Bethe roots $\{\tilde{u}_j^{(a)}\}$ for the ground state have the form

$$\left\{ \begin{array}{lcl} v_j^{(a,1)} & : & j = 1\,, 2\,, \ldots\,, M_{(a,1)} \\ v_j^{(a,2)} + \frac{i\pi}{2}\,, & : & j = 1\,, 2\,, \ldots\,, M_{(a,2)} \end{array} \right. , \qquad a = 1\,, 2\,, \tag{4.51}$$

where $\{v_j^{(a,b)}\}$ are all real and positive; also, $M_{(1,1)} = M_{(2,1)} = \frac{N}{2}$, and $M_{(1,2)} = \frac{p+1}{2}$, $M_{(2,2)} = \frac{p-1}{2}$. Evidently there are two "seas" of real roots, namely $\{v_j^{(1,1)}\}$ and $\{v_j^{(2,1)}\}$.

We now proceed to compute the boundary energy, using notations similar to those in Case I. Defining

$$v_j^{(a,b)} = \mu \lambda_j^{(a,b)}\,, \tag{4.52}$$

the Bethe Ansatz equations (4.47), (4.48) for the sea roots are

$$e_1(\lambda_j^{(1,1)})^{2N+1} \quad = \quad -\left[g_1(\lambda_j^{(1,1)}) e_{1+2a_-}(\lambda_j^{(1,1)}) e_{1-2a_-}(\lambda_j^{(1,1)}) e_{1+2a_+}(\lambda_j^{(1,1)}) e_{1-2a_+}(\lambda_j^{(1,1)})\right]$$

[19]The periodicity and crossing properties of $Q_a(u)$ imply that the zeros $u_j^{(a)}$ are defined up to $u_j^{(a)} \mapsto u_j^{(a)} + i\pi$ and $u_j^{(a)} \mapsto -u_j^{(a)} - \eta$, which corresponds to $\tilde{u}_j^{(a)} \mapsto \tilde{u}_j^{(a)} + i\pi$ and $\tilde{u}_j^{(a)} \mapsto -\tilde{u}_j^{(a)}$, respectively. We use these symmetries to restrict the roots to the fundamental region $\Re e\, \tilde{u}_j^{(a)} \geq 0$ and $-\frac{\pi}{2} < \Im m\, \tilde{u}_j^{(a)} \leq \frac{\pi}{2}$.

$$\times \prod_{k=1}^{N/2} \left[e_2(\lambda_j^{(1,1)} - \lambda_k^{(2,1)}) e_2(\lambda_j^{(1,1)} + \lambda_k^{(2,1)}) \right]$$
$$\times \prod_{k=1}^{(p-1)/2} \left[g_2(\lambda_j^{(1,1)} - \lambda_k^{(2,2)}) g_2(\lambda_j^{(1,1)} + \lambda_k^{(2,2)}) \right] , \qquad (4.53)$$

and

$$e_1(\lambda_j^{(2,1)})^{2N+1} g_1(\lambda_j^{(2,1)})^{-1}$$
$$= - \prod_{k=1}^{N/2} \left[e_2(\lambda_j^{(2,1)} - \lambda_k^{(1,1)}) e_2(\lambda_j^{(2,1)} + \lambda_k^{(1,1)}) \right]$$
$$\times \prod_{k=1}^{(p+1)/2} \left[g_2(\lambda_j^{(2,1)} - \lambda_k^{(1,2)}) g_2(\lambda_j^{(2,1)} + \lambda_k^{(1,2)}) \right] , \qquad (4.54)$$

respectively, where $j = 1 , \ldots , \frac{N}{2}$. The corresponding ground-state counting functions are

$$\mathsf{h}^{(1)}(\lambda) = \frac{1}{2\pi} \Big\{ (2N+1) q_1(\lambda) - r_1(\lambda) - q_{1+2a_-}(\lambda) - q_{1-2a_-}(\lambda) - q_{1+2a_+}(\lambda) - q_{1-2a_+}(\lambda)$$
$$- \sum_{k=1}^{N/2} \left[q_2(\lambda - \lambda_k^{(2,1)}) + q_2(\lambda + \lambda_k^{(2,1)}) \right] - \sum_{k=1}^{(p-1)/2} \left[r_2(\lambda - \lambda_k^{(2,2)}) + r_2(\lambda + \lambda_k^{(2,2)}) \right] \Big\} , \qquad (4.55)$$

and

$$\mathsf{h}^{(2)}(\lambda) = \frac{1}{2\pi} \Big\{ (2N+1) q_1(\lambda) - r_1(\lambda)$$
$$- \sum_{k=1}^{N/2} \left[q_2(\lambda - \lambda_k^{(1,1)}) + q_2(\lambda + \lambda_k^{(1,1)}) \right] - \sum_{k=1}^{(p+1)/2} \left[r_2(\lambda - \lambda_k^{(1,2)}) + r_2(\lambda + \lambda_k^{(1,2)}) \right] \Big\} . \qquad (4.56)$$

Repeating the maneuver (4.23) in the summations over the sea roots, and letting N become large, we obtain a pair of coupled linear integral equations for the ground-state root densities $\rho^{(a)}(\lambda)$,

$$\rho^{(1)}(\lambda) = \frac{1}{N} \frac{d\mathsf{h}^{(1)}}{d\lambda} = 2a_1(\lambda) - \int_{-\infty}^{\infty} d\lambda' \ a_2(\lambda - \lambda') \ \rho^{(2)}(\lambda')$$
$$+ \frac{1}{N} \Big\{ a_1(\lambda) + a_2(\lambda) - b_1(\lambda) - a_{1+2a_-}(\lambda) - a_{1-2a_-}(\lambda)$$

$$- \quad a_{1+2a_+}(\lambda) - a_{1-2a_+}(\lambda) - \sum_{k=1}^{(p-1)/2} \Big[b_2(\lambda - \lambda_k^{(2,2)}) + b_2(\lambda + \lambda_k^{(2,2)}) \Big] \Big\} , \tag{4.57}$$

and

$$\begin{aligned} \rho^{(2)}(\lambda) &= \frac{1}{N} \frac{d\mathsf{h}^{(2)}}{d\lambda} = 2a_1(\lambda) - \int_{-\infty}^{\infty} d\lambda' \ a_2(\lambda - \lambda') \ \rho^{(1)}(\lambda') \\ &+ \frac{1}{N} \Big\{ a_1(\lambda) + a_2(\lambda) - b_1(\lambda) - \sum_{k=1}^{(p+1)/2} \Big[b_2(\lambda - \lambda_k^{(1,2)}) + b_2(\lambda + \lambda_k^{(1,2)}) \Big] \Big\} . \end{aligned} \tag{4.58}$$

It is straightforward to solve by Fourier transforms for the individual root densities. However, we shall see that the energy depends only on the sum of the root densities, which is given by

$$\rho^{(1)}(\lambda) + \rho^{(2)}(\lambda) = 4s(\lambda) + \frac{1}{N} \mathcal{R}(\lambda) , \tag{4.59}$$

where

$$\begin{aligned} \hat{\mathcal{R}}(\omega) &= \frac{1}{1 + \hat{a}_2(\omega)} \Big\{ 2\hat{a}_1(\omega) + 2\hat{a}_2(\omega) - 2\hat{b}_1(\omega) - \hat{a}_{1+2a_-}(\omega) - \hat{a}_{1-2a_-}(\omega) \\ &- \hat{a}_{1+2a_+}(\omega) - \hat{a}_{1-2a_+}(\omega) - 2 \sum_{a=1}^{2} \sum_{k=1}^{M_{(a,2)}} \cos(\omega \lambda_k^{(a,2)}) \ \hat{b}_2(\omega) \Big\} . \end{aligned} \tag{4.60}$$

The expression (4.49) for the energy and the string hypothesis (4.50) imply

$$\begin{aligned} E &= -\frac{1}{2} \sinh^2 \eta \Big\{ - \sum_{a=1}^{2} \sum_{j=1}^{N/2} \frac{1}{\sinh(v_j^{(a,1)} - \frac{\eta}{2}) \sinh(v_j^{(a,1)} + \frac{\eta}{2})} \\ &- \sum_{a=1}^{2} \sum_{j=1}^{M_{(a,2)}} \frac{1}{\cosh(v_j^{(a,2)} - \frac{\eta}{2}) \cosh(v_j^{(a,2)} + \frac{\eta}{2})} \Big\} + \frac{1}{2}(N-1) \cosh \eta \\ &= -\frac{\pi \sin \mu}{\mu} \Big\{ \sum_{a=1}^{2} \sum_{j=1}^{N/2} a_1(\lambda_j^{(a,1)}) + \sum_{a=1}^{2} \sum_{j=1}^{M_{(a,2)}} b_1(\lambda_j^{(a,2)}) \Big\} + \frac{1}{2}(N-1) \cos \mu \\ &= -\frac{\pi \sin \mu}{\mu} \Big\{ \frac{1}{2} \sum_{a=1}^{2} \sum_{j=-N/2}^{N/2} a_1(\lambda_j^{(a,1)}) - a_1(0) + \sum_{a=1}^{2} \sum_{j=1}^{M_{(a,2)}} b_1(\lambda_j^{(a,2)}) \Big\} \\ &+ \frac{1}{2}(N-1) \cos \mu \end{aligned}$$

$$
\begin{aligned}
&= -\frac{\pi \sin\mu}{\mu}\Big\{\frac{N}{2}\int_{-\infty}^{\infty} d\lambda\ a_1(\lambda)\left[\rho^{(1)}(\lambda)+\rho^{(2)}(\lambda)\right] - a_1(0) \\
&\quad + \sum_{a=1}^{2}\sum_{j=1}^{M_{(a,2)}} b_1(\lambda_j^{(a,2)})\Big\} + \frac{1}{2}(N-1)\cos\mu\,. \qquad (4.61)
\end{aligned}
$$

Substituting the result (4.59) for the sum of the root densities, we obtain

$$
E = E_{bulk} + E_{boundary}\,, \qquad (4.62)
$$

where the bulk (order N) energy is again given by (4.35), and the boundary (order 1) energy is given by

$$
E_{boundary} = -\frac{\pi \sin\mu}{\mu}\Big\{\mathcal{I} + \sum_{a=1}^{2}\sum_{j=1}^{M_{(a,2)}} b_1(\lambda_j^{(a,2)})\Big\} - \frac{1}{2}\cos\mu\,, \qquad (4.63)
$$

where $\mathcal{I}$ is the integral

$$
\begin{aligned}
\mathcal{I} &= \frac{1}{2}\int_{-\infty}^{\infty} d\lambda\ a_1(\lambda)\left[\mathcal{R}(\lambda) - 2\delta(\lambda)\right] = \frac{1}{4\pi}\int_{-\infty}^{\infty} d\omega\ \hat{a}_1(\omega)\left[\hat{\mathcal{R}}(\omega) - 2\right] \\
&= -\sum_{a=1}^{2}\sum_{j=1}^{M_{(a,2)}} b_1(\lambda_j^{(a,2)}) + \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\ \hat{s}(\omega)\Big\{\hat{a}_1(\omega) - \hat{b}_1(\omega) - 1 \\
&\quad -\frac{1}{2}\left[\hat{a}_{1+2a_-}(\omega) + \hat{a}_{1-2a_-}(\omega) + \hat{a}_{1+2a_+}(\omega) + \hat{a}_{1-2a_+}(\omega)\right]\Big\}\,. \qquad (4.64)
\end{aligned}
$$

Once again there is a remarkable cancellation among terms involving Bethe roots which are not parts of the seas, namely, $\lambda_j^{(a,2)}$. Writing $E_{boundary}$ as the sum of contributions from the left and right boundaries, we conclude that for the parameter values [20]

$$
\frac{1}{2} \le |a_\pm| < \nu - \frac{1}{2}\,, \qquad (4.65)
$$

the energy contribution from each boundary is given by

$$
\begin{aligned}
E^{\pm}_{boundary} &= -\frac{\sin\mu}{2\mu}\int_{-\infty}^{\infty} d\omega\ \frac{1}{2\cosh(\omega/2)}\Big\{\frac{\cosh((\nu-2)\omega/4)}{2\cosh(\nu\omega/4)} - \frac{1}{2} \\
&\quad + \frac{\sinh(\omega/2)\cosh((\nu-2|a_\pm|)\omega/2)}{\sinh(\nu\omega/2)}\Big\} - \frac{1}{4}\cos\mu\,. \qquad (4.66)
\end{aligned}
$$

[20] This restriction arises when using the Fourier transform result (4.30) to evaluate $\hat{a}_{1+2a_\pm}(\omega) + \hat{a}_{1-2a_\pm}(\omega)$.

This result agrees with the result (4.4) with $b_\pm = 0$ and $a_\pm$ values (4.65). As shown in Appendix 3, the integrals (with p odd) can also be evaluated analytically.

We have derived the above result for the boundary energy under the assumption that the Bethe roots for the ground state have the form (4.50), which is true only for suitable values of the boundary parameters $a_\pm$, namely,

$$\frac{\nu - 1}{2} < |a_\pm| < \frac{\nu + 1}{2}\,, \qquad a_+ a_- > 0\,, \tag{4.67}$$

where $\nu = p + 1$. For parameter values outside the region (4.67), one or more of the Bethe roots has an imaginary part which is *not* a multiple of $\pi/2$ and which evidently depends on the parameter values. One can verify that the region (4.67) is contained in the region (4.65).

As in Case I, it is possible to give a qualitative explanation of the restriction (4.67) by a heuristic argument. Indeed, let us rewrite the Hamiltonian (4.41) as

$$\mathcal{H} = \mathcal{H}_0 + h_1^x \sigma_1^x + h_N^x \sigma_N^x\,, \tag{4.68}$$

where the boundary magnetic fields are given by

$$h_1^x = \frac{1}{2}\sinh\eta\,\mathrm{cosech}\,\alpha_-\,, \quad h_N^x = \frac{1}{2}\sinh\eta\,\mathrm{cosech}\,\alpha_+\,. \tag{4.69}$$

For $\alpha_\pm \approx i\pi/2$ or $-i\pi/2$ (i.e., $a_\pm \approx \nu/2$ or $-\nu/2$), the boundary magnetic fields in the x direction are small and parallel. Hence, the ground state and corresponding Bethe roots are "simple." Outside of this region of parameter space, the boundary fields in the x direction are large and/or antiparallel, and so the ground state and corresponding Bethe roots are "complicated."

We have investigated the ground state of the open XXZ spin chain with nondiagonal boundary terms which are parametrized by pairs of boundary parameters, in the thermodynamic limit, using the new exact solutions [51, 52] and the string hypothesis. This investigation has revealed some surprises. Indeed, for Case I

(4.2), the ground state is described in part by a sea of strings of length 2 (4.17), which is characteristic of spin-1 chains [58]. For Case II (4.3), the energy depends on two sets of Bethe roots (4.49), and in fact on the sum of the corresponding root densities (4.61). For each case, there is a remarkable cancellation of the energy contributions from non-sea Bethe roots.

Perhaps the biggest surprise is that, for the two cases studied here, the boundary energies coincide with the result (4.4) for the constrained case (2.3), even when that constraint is not satisfied. This suggests that the result (4.4) may hold for general values of the boundary parameters.

Chapter 5: Boundary Energy of The General Open XXZ Chain at Roots of Unity

As is well known, for both the closed chain and the open chain with diagonal boundary terms, the eigenvalues of the Hamiltonian (and more generally, the transfer matrix) can be expressed in terms of zeros ("Bethe roots") of a single function $Q(u)$. This is in sharp contrast with the solution [53], which involves multiple Q functions, and therefore, multiple sets of Bethe roots. The number of such Q functions depends on the value of p. (Generalized $T-Q$ equations involving two such Q functions first arose in [52] for special values of the boundary parameters.)

The solution [60] has additional properties which distinguish it from typical Bethe Ansatz solutions: the Q functions also have normalization constants which must be determined; and the Bethe Ansatz equations have a nonconventional form. Given the unusual nature of this solution, one can justifiably wonder whether it provides a practical means of computing properties of the chain in the thermodynamic ($N \to \infty$) limit. To address this question, we set out to compute the so-called boundary or surface energy (i.e., the order 1 contribution to the ground-state energy), which is perhaps the most accessible boundary-dependent quantity. For the case of diagonal boundary terms, this quantity was first computed numerically in [15], and then analytically in [57].

We find that the boundary energy computation is indeed feasible. The key point is that, when the boundary parameters are in some suitable domain, the ground-state Bethe roots appear to follow certain remarkable patterns. By assuming the strict validity of these patterns ("string hypothesis"), the Bethe equations reduce to a conventional form. Hence, standard techniques can then be used to complete the computation. We find that our final result (5.44) for the boundary energy coincides with the result obtained in [42] for the case that the boundary parameters obey the constraint (2.3), and in [53] for special values [51, 52] of the boundary parameters at roots of unity.

5.1 Bethe Ansatz

In this section, we briefly recall the Bethe Ansatz solution [60]. In order to ensure hermiticity of the Hamiltonian (1.1), we take the boundary parameters $\beta_\pm$ real; $\alpha_\pm$ imaginary; $\theta_\pm$ imaginary. We begin by introducing the Ansatz for the various $Q(u)$ functions that appear in our solution, which we denote as $a_j(u)$ and $b_j(u)$:

$$\begin{aligned} a_j(u) &= A_j \prod_{k=1}^{2M_a} \sinh(u - u_k^{(a_j)})\,, \qquad b_j(u) = B_j \prod_{k=1}^{2M_b} \sinh(u - u_k^{(b_j)})\,, \\ & \qquad j = 1\,, \ldots\,, \lfloor \frac{p+1}{2} \rfloor\,, \end{aligned} \tag{5.1}$$

where $\{u_k^{(a_j)}\,, u_k^{(b_j)}\}$ are the zeros of $a_j(u)$ and $b_j(u)$ respectively, and $\lfloor\ \rfloor$ denotes integer part. If p is even, then there is one additional set of functions corresponding to $j = \frac{p}{2} + 1$,

$$\begin{aligned} a_{\frac{p}{2}+1}(u) &= A_{\frac{p}{2}+1} \prod_{k=1}^{M_a} \sinh(u - u_k^{(a_{\frac{p}{2}+1})}) \sinh(u + u_k^{(a_{\frac{p}{2}+1})})\,, \\ b_{\frac{p}{2}+1}(u) &= B_{\frac{p}{2}+1} \prod_{k=1}^{M_b} \sinh(u - u_k^{(b_{\frac{p}{2}+1})}) \sinh(u + u_k^{(b_{\frac{p}{2}+1})})\,. \end{aligned} \tag{5.2}$$

The normalization constants $\{A_j\,, B_j\}$ are yet to be determined [21]. We assume that N is even, in which case the integers $M_a\,, M_b$ are given by

$$M_a = \frac{N}{2} + 2p\,, \qquad M_b = \frac{N}{2} + p - 1\,, \tag{5.3}$$

[21] One of these normalization constants can be set to unity.

It is clear from (5.1), (5.2) that $a_j(u)$ and $b_j(u)$ have the following periodicity and crossing properties,

$$\begin{aligned} a_j(u+i\pi) &= a_j(u)\,, \qquad b_j(u+i\pi) = b_j(u)\,, \qquad j=1\,,\ldots\,,\lfloor\frac{p}{2}\rfloor+1\,, &(5.4)\\ a_{\frac{p}{2}+1}(-u) &= a_{\frac{p}{2}+1}(u)\,, \qquad b_{\frac{p}{2}+1}(-u) = b_{\frac{p}{2}+1}(u)\,. &(5.5)\end{aligned}$$

The zeros of the functions $\{a_j(u)\}$ and $\{b_j(u)\}$ satisfy the following Bethe Ansatz equations

$$\frac{h_0(-u_l^{(a_1)}-\eta)}{h_0(u_l^{(a_1)})} = -\frac{f_1(u_l^{(a_1)})\ a_1(-u_l^{(a_1)})+g_1(u_l^{(a_1)})\ Y(u_l^{(a_1)})^2\ b_1(-u_l^{(a_1)})}{2a_2(u_l^{(a_1)})\ h_1(-u_l^{(a_1)}-\eta)\ \prod_{k=1}^{p} h_1(u_l^{(a_1)}+k\eta)} \tag{5.6}$$

$$\frac{h(-u_l^{(a_j)}-j\eta)}{h(u_l^{(a_j)}+(j-1)\eta)} = -\frac{a_{j-1}(u_l^{(a_j)})}{a_{j+1}(u_l^{(a_j)})}\,, \qquad j=2\,,\ldots\,,\lfloor\frac{p}{2}\rfloor+1\,, \tag{5.7}$$

and

$$\frac{h_0(-u_l^{(b_1)}-\eta)}{h_0(u_l^{(b_1)})} = -\frac{f_1(u_l^{(b_1)})\ b_1(-u_l^{(b_1)})+g_1(u_l^{(b_1)})\ a_1(-u_l^{(b_1)})}{2b_2(u_l^{(b_1)})\ h_1(-u_l^{(b_1)}-\eta)\ \prod_{k=1}^{p} h_1(u_l^{(b_1)}+k\eta)}\,, \tag{5.8}$$

$$\frac{h(-u_l^{(b_j)}-j\eta)}{h(u_l^{(b_j)}+(j-1)\eta)} = -\frac{b_{j-1}(u_l^{(b_j)})}{b_{j+1}(u_l^{(b_j)})}\,, \qquad j=2\,,\ldots\,,\lfloor\frac{p}{2}\rfloor+1\,, \tag{5.9}$$

where $a_{\frac{p}{2}+2}(u) = a_{\frac{p}{2}}(-u)$ and $a_{\frac{p+3}{2}}(u) = a_{\frac{p+1}{2}}(-u)$ for even and odd values of p, respectively, and similarly for the b's. Moreover,

$$h(u) = h_0(u)\ h_1(u)\,, \tag{5.10}$$

where $h_0(u)$ and $h_1(u)$ are as follows

$$\begin{aligned} h_0(u) &= \sinh^{2N}(u+\eta)\frac{\sinh(2u+2\eta)}{\sinh(2u+\eta)}\,,\\ h_1(u) &= -4\sinh(u+\alpha_-)\cosh(u+\beta_-)\sinh(u+\alpha_+)\cosh(u+\beta_+)\,. &(5.11)\end{aligned}$$

We also define the quantities

$$g_1(u) = 2\sinh(2(p+1)u) \tag{5.12}$$

and

$$Y(u)^2 = \sum_{k=0}^{2} \mu_k \cosh^k(2(p+1)u)\,. \tag{5.13}$$

Explicit expressions for the coefficients μ_k in (5.13), which depend on the boundary parameters, are listed in the Appendix 2 for both even and odd values of p. The function $f_1(u)$ for even and odd p are given by (2.22) and (2.24) respectively.

Moreover, there are additional Bethe-Ansatz-like equations

$$a_1(\frac{\eta}{2}) = a_2(-\frac{\eta}{2})\,, \tag{5.14}$$

$$a_{j-1}((\frac{1}{2}-j)\eta) = a_{j+1}((\frac{1}{2}-j)\eta)\,, \qquad j=2\,,\ldots\,,\lfloor\frac{p}{2}\rfloor+1\,, \tag{5.15}$$

which relate the normalization constants $\{A_j\}$; and also

$$b_1(\frac{\eta}{2}) = b_2(-\frac{\eta}{2})\,, \tag{5.16}$$

$$b_{j-1}((\frac{1}{2}-j)\eta) = b_{j+1}((\frac{1}{2}-j)\eta)\,, \qquad j=2\,,\ldots\,,\lfloor\frac{p}{2}\rfloor+1\,, \tag{5.17}$$

which relate the normalization constants $\{B_j\}$. There are also equations that relate the normalization constants A_1 and B_1, such as

$$f_1(-\alpha_- - \eta)\; b_1(\alpha_- + \eta) = -g_1(-\alpha_- - \eta)\; a_1(\alpha_- + \eta)\,. \tag{5.18}$$

The energy eigenvalues of the Hamiltonian (2.1) are given by

$$E = \frac{1}{2}\sinh\eta \sum_{l=1}^{2M_b} \left[\coth(u_l^{(b_j)} + (j-1)\eta) - \coth(u_l^{(b_{j-1})} + (j-1)\eta)\right] + E_0\,,$$
$$j = 2\,,\ldots\,,\lfloor\frac{p+1}{2}\rfloor\,, \tag{5.19}$$

where E_0 is defined as

$$E_0 = \frac{1}{2}\sinh\eta\,(\coth\alpha_- + \tanh\beta_- + \coth\alpha_+ + \tanh\beta_+) + \frac{1}{2}(N-1)\cosh\eta\,. \tag{5.20}$$

For even p, there is one more expression for the energy corresponding to $j=\frac{p}{2}+1$,

$$E = \frac{1}{2}\sinh\eta\Bigg\{\sum_{l=1}^{M_b}\left[\coth(u_l^{(b_{\frac{p}{2}+1})} + \frac{p\eta}{2}) - \coth(u_l^{(b_{\frac{p}{2}+1})} - \frac{p\eta}{2})\right]$$
$$- \sum_{l=1}^{2M_b}\coth(u_l^{(b_{\frac{p}{2}})} + \frac{p\eta}{2})\Bigg\} + E_0\,. \tag{5.21}$$

There are also similar expressions for the energy in terms of a roots $\{u_l^{(a_j)}\}$ [60].

5.2 Even p

In this section, we consider the case where the bulk anisotropy parameter assumes the values (2.70), $\eta = \frac{i\pi}{3}, \frac{i\pi}{5}, \ldots$. We have studied the Bethe roots corresponding to the ground state numerically for small values of p and N along the lines of [28]. We have found that, when the boundary parameters are in some suitable domain (which we discuss further below Eq. (5.44)), the ground state Bethe roots $\{u_k^{(a_j)}, u_k^{(b_j)}\}$ have a remarkable pattern. An example with $p = 2\,, N = 4$ is shown in Figure 5.1. Specifically, these roots can be categorized into "sea" roots, $\{v_k^{\pm(a_j)}, v_k^{\pm(b_j)}\}$ (the number of which depends on N) and the remaining "extra" roots, $\{w_k^{\pm(a_j,l)}, w_k^{\pm(b_j)}\}$ (the number of which depends on p) according to the following pattern which we adopt as our "string hypothesis."

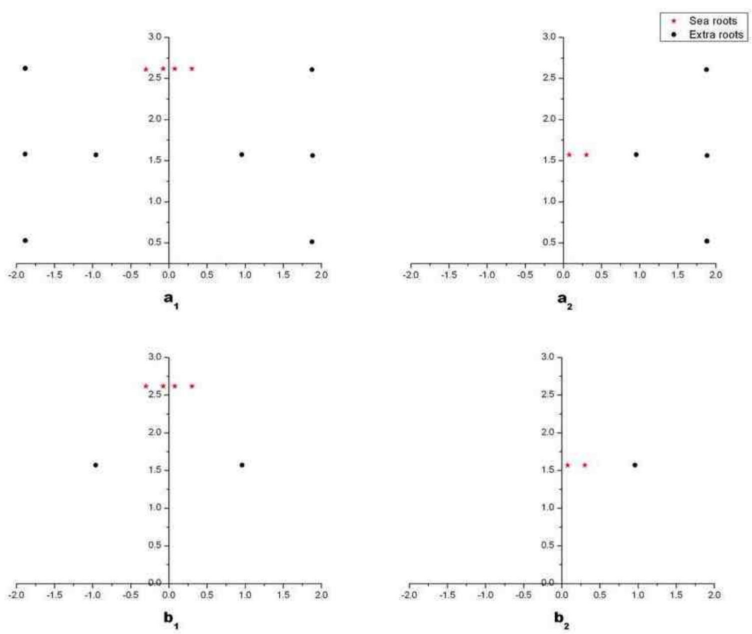

Figure 5.1: Ground-state Bethe roots for $p = 2$, $N = 4$, $\alpha_- = 0.604i$, $\alpha_+ = 0.535i$, $\beta_- = -1.882$, $\beta_+ = 1.878$, $\theta_- = 0.6i$, $\theta_+ = 0.7i$.

5.2.1 Sea roots $\{v_k^{\pm(a_j)}\,, v_k^{\pm(b_j)}\}$

Sea roots of all $\{a_j(u)\,, b_j(u)\}$ functions for any even p are summarized below,

$$\begin{aligned} v_k^{\pm(a_j)} &= v_k^{\pm(b_j)} = \pm\tilde{v}_k + \left(\frac{2p+3-2j}{2}\right)\eta\,, \quad k = 1\,, \ldots\,, \frac{N}{2}\,, \\ & j = 1\,, \ldots\,, \frac{p}{2}+1\,, \end{aligned} \tag{5.22}$$

where $\tilde{v}_k$ are real and positive. In Figure 5.1, the sea roots are indicated with red stars.

Note that the real parts $(\pm\tilde{v}_k)$ are independent of j. This, as we shall see, greatly simplifies the analysis. Furthermore, for each sea root with real part $+\tilde{v}_k$, there is an additional "mirror" sea root with real part $-\tilde{v}_k$, for a total of N sea roots, provided $j \neq \frac{p}{2}+1$. For $j = \frac{p}{2}+1$, there are only $\frac{N}{2}$ sea roots $+\tilde{v}_k + \frac{i\pi}{2}$ (i.e., just the root with positive real part) due to the crossing symmetry (5.5) of the functions $a_{\frac{p}{2}+1}(u)$ and $b_{\frac{p}{2}+1}(u)$. [22]

5.2.2 Extra roots $\{w_k^{\pm(a_j,l)}\,, w_k^{\pm(b_j)}\}$

We next describe the remaining extra Bethe roots for even p, the number of which depends on the value of p. In Figure 5.1, the extra roots are indicated with black circles. Since the functions $a_j(u)$ and $b_j(u)$ have a different number of such extra roots, we present them separately. The extra roots of the $b_j(u)$ functions have the form

$$\begin{aligned} w_k^{\pm(b_j)} &= \pm\tilde{w}_k + \left(\frac{2p+1-2k}{2}\right)\eta\,, \quad k = 1\,, \ldots\,, p-1\,, \\ & j = 1\,, \ldots\,, \frac{p}{2}+1\,. \end{aligned} \tag{5.23}$$

[22] Hence, strictly speaking, we should write the $j = \frac{p}{2}+1$ equation in (5.22) separately, keeping only the + roots. However, in order to avoid doubling the number of equations, we commit this abuse of notation here and throughout this section.

The real parts of the roots, $\tilde{w}_k$, are not all independent. Instead, they are related to each other pairwise as follows,

$$\tilde{w}_k = \tilde{w}_{p-k}\,, \qquad k = 1\,, \ldots\,, \frac{p}{2} - 1\,. \tag{5.24}$$

Only $\tilde{w}_{\frac{p}{2}}$ remains unpaired. This property proves to be crucial for the boundary energy calculation.

There are two types of extra roots of the $a_j(u)$ functions:

$$\begin{aligned} w_k^{\pm(a_j,1)} &= w_k^{\pm(b_j)} = \pm\tilde{w}_k + \left(\frac{2p+1-2k}{2}\right)\eta\,, \quad k = 1\,, \ldots\,, p-1\,, \\ w_k^{\pm(a_j,2)} &= \pm\tilde{w}_0 + \left(\frac{2p+3-2k}{2}\right)\eta\,, \quad k = 1\,, \ldots\,, p+1\,, \\ & \qquad j = 1\,, \ldots\,, \frac{p}{2} + 1\,. \end{aligned} \tag{5.25}$$

Note that the extra roots of the first type $\{w_k^{\pm(a_j,1)}\}$ coincide with the b roots $\{w_k^{\pm(b_j)}\}$; and that the extra roots of the second type $\{w_k^{\pm(a_j,2)}\}$ form a "$(p+1)$-string", with real part $\tilde{w}_0$.

As previously remarked, for $j = \frac{p}{2} + 1$, only the roots with the $+$ sign appear.

5.2.3 Boundary energy

We now proceed to compute the boundary energy. Using the expression (5.19) for the energy and our string hypothesis, we obtain (for $p > 2$)

$$\begin{aligned} E &= \frac{1}{2}\sinh\eta\Bigg\{\sum_{k=1}^{\frac{N}{2}}\Big[\coth(v_k^{+(b_j)} + (j-1)\eta) + \coth(v_k^{-(b_j)} + (j-1)\eta) \\ &- \coth(v_k^{+(b_{j-1})} + (j-1)\eta) - \coth(v_k^{-(b_{j-1})} + (j-1)\eta)\Big] \\ &+ \sum_{k=1}^{p-1}\Big[\coth(w_k^{+(b_j)} + (j-1)\eta) + \coth(w_k^{-(b_j)} + (j-1)\eta) \\ &- \coth(w_k^{+(b_{j-1})} + (j-1)\eta) - \coth(w_k^{-(b_{j-1})} + (j-1)\eta)\Big]\Bigg\} + E_0\,, \\ & \qquad j = 2\,, \ldots\,, \frac{p}{2}\,. \end{aligned} \tag{5.26}$$

Recalling (5.22) and (5.23), this expression for the energy reduces to

$$E = \sinh^2\eta \sum_{k=1}^{\frac{N}{2}} \frac{1}{\sinh(\tilde{v}_k - \frac{\eta}{2})\sinh(\tilde{v}_k + \frac{\eta}{2})} + E_0\,, \quad \tilde{v}_k > 0\,, \tag{5.27}$$

independently of the value of j. Since the extra roots $w_k^{(b_j)}$ are independent of j, their contribution to the energy evidently cancels, leaving only the sea-root terms in (5.27). The same result can also be obtained (for $p \geq 2$) from the energy expression (5.21).

We turn now to the Bethe Ansatz equations, on which we must also impose our string hypothesis. Choosing $j = \frac{p}{2}+1$ in (5.9) with $u_l^{(b_j)}$ equal to the sea root $v_l^{+(b_{\frac{p}{2}+1})} = \tilde{v}_l + \frac{i\pi}{2}$, we obtain

$$\frac{h(-\tilde{v}_l - \frac{\eta}{2})}{h(\tilde{v}_l - \frac{\eta}{2})} = -\frac{b_{\frac{p}{2}}(\tilde{v}_l + \frac{i\pi}{2})}{b_{\frac{p}{2}}(-\tilde{v}_l - \frac{i\pi}{2})}\,, \tag{5.28}$$

where we have made use of the fact $b_{\frac{p}{2}+2}(u) = b_{\frac{p}{2}}(-u)$. More explicitly, this equation reads

$$\begin{aligned}
&\left(\frac{\sinh(\tilde{v}_l + \frac{\eta}{2})}{\sinh(\tilde{v}_l - \frac{\eta}{2})}\right)^{2N} \frac{\sinh(2\tilde{v}_l + \eta)}{\sinh(2\tilde{v}_l - \eta)} \frac{\sinh(\tilde{v}_l - \frac{\eta}{2} + \alpha_-)}{\sinh(\tilde{v}_l + \frac{\eta}{2} - \alpha_-)} \frac{\cosh(\tilde{v}_l - \frac{\eta}{2} + \beta_-)}{\cosh(\tilde{v}_l + \frac{\eta}{2} - \beta_-)} \\
&\quad \times \frac{\sinh(\tilde{v}_l - \frac{\eta}{2} + \alpha_+)}{\sinh(\tilde{v}_l + \frac{\eta}{2} - \alpha_+)} \frac{\cosh(\tilde{v}_l - \frac{\eta}{2} + \beta_+)}{\cosh(\tilde{v}_l + \frac{\eta}{2} - \beta_+)} = -\prod_{k=1}^{\frac{N}{2}} \frac{\sinh(\tilde{v}_l - \tilde{v}_k + \eta)}{\sinh(\tilde{v}_l - \tilde{v}_k - \eta)} \frac{\sinh(\tilde{v}_l + \tilde{v}_k + \eta)}{\sinh(\tilde{v}_l + \tilde{v}_k - \eta)}\,, \\
&\qquad l = 1\,, \cdots\,, \frac{N}{2}\,, \quad \tilde{v}_k > 0\,.
\end{aligned} \tag{5.29}$$

In obtaining this result, we have made use of the fact that the normalization constant $B_{\frac{p}{2}}$ of the function $b_{\frac{p}{2}}(u)$ cancels, and also that the contribution from the extra roots on the RHS cancel as a consequence of the relation (5.24) among their real parts.

Remarkably, as a consequence of our string hypothesis, our non-conventional Bethe Ansatz equations have reduced to a conventional system (5.29), which can be analyzed by standard methods. However, before proceeding further with this computation, it is worth noting that the same equations can also be obtained starting from any $j > 1$. To see this, we first observe that the $\{A_j\}$ normalization constants are all equal, and similarly for the $\{B_j\}$ normalization constants,

$$A_1 = A_2 = \ldots = A_{\frac{p}{2}+1}\,, \qquad B_1 = B_2 = \ldots = B_{\frac{p}{2}+1}\,. \tag{5.30}$$

This result follows from the Bethe-Ansatz-like equations (5.14)-(5.17) and the string hypothesis. For example, using (5.22) and (5.23) in (5.16), and remembering the relation (5.24) among the real parts of the extra roots, we obtain $B_1 = B_2$. Hence, choosing $u_l^{(b_j)}$ in (5.9) to be a sea root $v_l^{+(b_j)}$ for any $j \in \{2\,, \ldots\,, \frac{p}{2}+1\}$, we again arrive at (5.29). Moreover, in view of the identity

$$\frac{a_{j-1}(v_l^{+(a_j)})}{a_{j+1}(v_l^{+(a_j)})} = \frac{b_{j-1}(v_l^{+(b_j)})}{b_{j+1}(v_l^{+(b_j)})}\,, \qquad j = 2\,, \ldots\,, \frac{p}{2}+1\,, \tag{5.31}$$

where $v_l^{+(a_j)} = v_l^{+(b_j)}$ is a sea root, the same result (5.29) can also be obtained from (3.45). [23]

In the thermodynamic ($N \to \infty$) limit, the number of sea roots becomes infinite. The distribution of the real parts of these roots $\{\tilde{v}_k\}$ can be represented by a density function, which is computed from the counting function. Using (4.20), we rewrite the Bethe Ansatz equations (5.29) in a more compact form,

$$\begin{aligned} e_1(\lambda_l)^{2N+1}\; g_1(\lambda_l)\frac{e_{2a_- -1}(\lambda_l)\; e_{2a_+ -1}(\lambda_l)}{g_{1+2ib_-}(\lambda_l)\; g_{1+2ib_+}(\lambda_l)} \quad &= \quad -\prod_{k=1}^{\frac{N}{2}} e_2(\lambda_l - \lambda_k)\; e_2(\lambda_l + \lambda_k)\,, \\ & \qquad l = 1\,, \cdots\,, \frac{N}{2}\,, \end{aligned} \tag{5.32}$$

where we have set $\tilde{v}_l = \mu\lambda_l$, $\eta = i\mu\,, \alpha_\pm = i\mu a_\pm\,, \beta_\pm = \mu b_\pm$. Note that the parameters μ, $a_\pm$, $b_\pm$ are all real.

Taking the logarithm of (5.32), we obtain the desired ground state counting function

$$\mathsf{h}(\lambda) \quad = \quad \frac{1}{2\pi}\Big\{(2N+1)q_1(\lambda) + r_1(\lambda) + q_{2a_- -1}(\lambda) - r_{1+2ib_-}(\lambda) + q_{2a_+ -1}(\lambda)$$

[23] Only the first set of Bethe equations (5.6), (5.8) do not seem to reduce to (5.29).

$$- \quad r_{1+2ib_+}(\lambda) - \sum_{k=1}^{\frac{N}{2}} \left[q_2(\lambda - \lambda_k) + q_2(\lambda + \lambda_k) \right] \Big\} \,, \tag{5.33}$$

where $q_n(\lambda)$ and $r_n(\lambda)$ are odd functions given by (4.22). Defining $\lambda_{-k} \equiv -\lambda_k$, we have

$$-\sum_{k=1}^{\frac{N}{2}} \left[q_2(\lambda - \lambda_k) + q_2(\lambda + \lambda_k) \right] = - \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} q_2(\lambda - \lambda_k) + q_2(\lambda) \,. \tag{5.34}$$

The root density $\rho(\lambda)$ for the ground state is therefore given by

$$\begin{aligned} \rho(\lambda) &= \frac{1}{N} \frac{d\mathsf{h}}{d\lambda} = 2a_1(\lambda) - \int_{-\infty}^{\infty} d\lambda' \ a_2(\lambda - \lambda') \ \rho(\lambda') + \frac{1}{N} \Big[a_1(\lambda) + b_1(\lambda) \\ &+ \ a_2(\lambda) + a_{2a_- -1}(\lambda) - b_{1+2ib_-}(\lambda) + a_{2a_+ -1}(\lambda) - b_{1+2ib_+}(\lambda) \Big] \,, \end{aligned} \tag{5.35}$$

where we have ignored corrections of higher order in $1/N$ when passing from a sum to an integral, and we have used (4.26) [24].

The solution of the linear integral equation (5.35) for $\rho(\lambda)$ is obtained by Fourier transforms and is given by

$$\rho(\lambda) = 2s(\lambda) + \frac{1}{N} R(\lambda) \,, \tag{5.36}$$

where

$$s(\lambda) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \ e^{-i\omega\lambda} \frac{1}{2\cosh(\omega/2)} = \frac{1}{2\cosh(\pi\lambda)} \,, \tag{5.37}$$

and

$$\begin{aligned} \hat{R}(\omega) &= \frac{1}{(1 + \hat{a}_2(\omega))} \Big\{ \hat{a}_1(\omega) + \hat{b}_1(\omega) + \hat{a}_2(\omega) - \hat{b}_{1+2ib_-}(\omega) - \hat{b}_{1+2ib_+}(\omega) \\ &+ \ \hat{a}_{2a_- -1}(\omega) + \hat{a}_{2a_+ -1}(\omega) \Big\} \,, \end{aligned} \tag{5.38}$$

with $\hat{a}_n(\omega)$ and $\hat{b}_n(\omega)$ given by (4.30) and (4.31) respectively.

[24] These new functions $a_n(\lambda)$ and $b_n(\lambda)$ should not be confused with the Q functions $a_j(u)$ and $b_j(u)$ appearing earlier.

Expressing the energy expression (5.27) in terms of the newly defined quantities and letting N become large, we obtain

$$\begin{aligned} E &= -\frac{2\pi \sin\mu}{\mu} \sum_{k=1}^{\frac{N}{2}} a_1(\lambda_k) + E_0 = -\frac{\pi \sin\mu}{\mu} \Big\{ \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} a_1(\lambda_k) - a_1(0) \Big\} + E_0 \\ &= -\frac{\pi \sin\mu}{\mu} \Big\{ N \int_{-\infty}^{\infty} d\lambda\ a_1(\lambda)\ \rho(\lambda) - a_1(0) \Big\} + \frac{1}{2}(N-1)\cos\mu \\ &+ \frac{1}{2}\sin\mu \left(\cot\mu a_- + i\tanh\mu b_- + \cot\mu a_+ + i\tanh\mu b_+\right) , \end{aligned} \tag{5.39}$$

where again we ignore corrections that are higher order in $1/N$. Substituting the result (5.36) for the root density, we obtain

$$E = E_{bulk} + E_{boundary} , \tag{5.40}$$

where the bulk (order N) energy is given by

$$\begin{aligned} E_{bulk} &= -\frac{2N\pi \sin\mu}{\mu} \int_{-\infty}^{\infty} d\lambda\ a_1(\lambda)\ s(\lambda) + \frac{1}{2} N\cos\mu \\ &= -N\sin^2\mu \int_{-\infty}^{\infty} d\lambda\ \frac{1}{[\cosh(2\mu\lambda) - \cos\mu]\cosh(\pi\lambda)} + \frac{1}{2}N\cos\mu , \end{aligned} \tag{5.41}$$

which agrees with the well-known result [13]. The boundary (order 1) energy is given by

$$\begin{aligned} E_{boundary} &= -\frac{\pi\sin\mu}{\mu} I - \frac{1}{2}\cos\mu + \frac{1}{2}\sin\mu \\ &\times \left(\cot\mu a_- + i\tanh\mu b_- + \cot\mu a_+ + i\tanh\mu b_+\right) , \end{aligned} \tag{5.42}$$

where I is the integral

$$\begin{aligned} I &= \int_{-\infty}^{\infty} d\lambda\ a_1(\lambda)\left[R(\lambda) - \delta(\lambda)\right] = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\ \hat{a}_1(\omega)\left[\hat{R}(\omega) - 1\right] \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\ \hat{s}(\omega)\Big\{\hat{a}_1(\omega) + \hat{b}_1(\omega) - 1 \\ &\quad -\hat{b}_{1+2ib_-}(\omega) - \hat{b}_{1+2ib_+}(\omega) + \hat{a}_{2a_- -1}(\omega) + \hat{a}_{2a_+ -1}(\omega)\Big\} . \end{aligned} \tag{5.43}$$

We further write the boundary energy as the sum of contributions from the left and right boundaries, $E_{boundary} = E^-_{boundary} + E^+_{boundary}$. The energy contribution from each boundary is given by

$$
\begin{aligned}
E^{\pm}_{boundary} &= -\frac{\sin\mu}{2\mu}\int_{-\infty}^{\infty} d\omega\ \frac{1}{2\cosh(\omega/2)}\Big\{\frac{\sinh((\nu-2)\omega/4)}{2\sinh(\nu\omega/4)} - \frac{1}{2} \\
&+ \operatorname{sgn}(2a_{\pm}-1)\frac{\sinh((\nu-|2a_{\pm}-1|)\omega/2)}{\sinh(\nu\omega/2)} + \frac{\sinh((2ib_{\pm}+1)\omega/2)}{\sinh(\nu\omega/2)}\Big\} \\
&+ \frac{1}{2}\sin\mu\,(\cot\mu a_{\pm} + i\tanh\mu b_{\pm}) - \frac{1}{4}\cos\mu\,. \qquad (5.44)
\end{aligned}
$$

This result can be shown to coincide with previous results in [42, 53], namely (4.4) and (4.38).

We emphasize that the result (5.44) has been derived under the assumption that the Bethe roots for the ground state obey the string hypothesis, which is true only for suitable values of the boundary parameters. For example, the shaded areas in Figures 5.2 and 5.3 denote regions of parameter space for which the ground-state Bethe roots have the form described in Sections 5.2.1 and 5.2.2. The $\alpha_{\pm}$ and $\beta_{\pm}$ parameters are varied in the two figures, respectively.

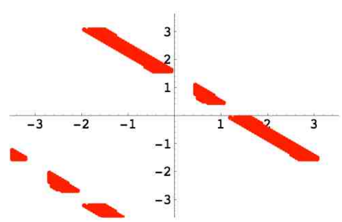

Figure 5.2: Shaded area denotes region of the $(\Im m\,\alpha_{+}\,, \Im m\,\alpha_{-})$ plane for which the ground-state Bethe roots obey the string hypothesis for $p=2$, $N=2$, $\beta_{-}=-1.882$, $\beta_{+}=1.878$, $\theta_{-}=0.6i$, $\theta_{+}=0.7i$.

5.3 Odd p

In this section, we consider the case where the bulk anisotropy parameter assumes the values (2.70) with p odd, i.e., $\eta = \frac{i\pi}{2}\,, \frac{i\pi}{4}\,, \ldots$. As for the even p case, for suitable values of the boundary parameters, the ground state Bethe roots $\{u_k^{(a_j)}, u_k^{(b_j)}\}$ have a regular pattern. An example with $p=3\,, N=4$ is shown in

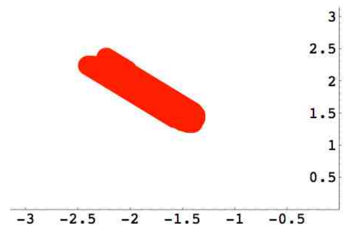

Figure 5.3: Shaded area denotes region of the (β_+, β_-) plane for which the ground-state Bethe roots obey the string hypothesis for $p = 2$, $N = 2$, $\alpha_- = -1.818i$, $\alpha_+ = 2.959i$, $\theta_- = 0.7i$, $\theta_+ = 0.6i$.

Figure 5.4. As before, these roots can be categorized into sea roots (the number of which depends on N) and extra roots (the number of which depends on p) according to the following pattern which we adopt as our "string hypothesis."

5.3.1 Sea roots $\{v_k^{\pm(a_j)}, v_k^{\pm(b_j)}\}$

Sea roots of all $\{a_j(u), b_j(u)\}$ functions for odd p are given by

$$v_k^{\pm(a_j)} = v_k^{\pm(b_j)} = \pm\tilde{v}_k + \left(\frac{2p+3-2j}{2}\right)\eta, \quad k = 1, \ldots, \frac{N}{2}, \quad j = 1, \ldots, \frac{p+1}{2}, \tag{5.45}$$

where $\tilde{v}_k$ are real and positive. In Figure 5.4, the sea roots are indicated with red stars.

As in the even p case, the real parts $(\pm\tilde{v}_k)$ are independent of j. This again provides simplification to the analysis. In contrast to the even p case, now none of the functions $\{a_j(u), b_j(u)\}$ has crossing symmetry. Hence, there are N sea roots for all values of j.

5.3.2 Extra roots $\{w_k^{(a_j,l)}, w_k^{(b_j)}\}$

We now describe the extra Bethe roots for odd p. In Figure 5.4, the extra roots are indicated with black circles. We start with the $p-1$ extra roots of the $b_j(u)$

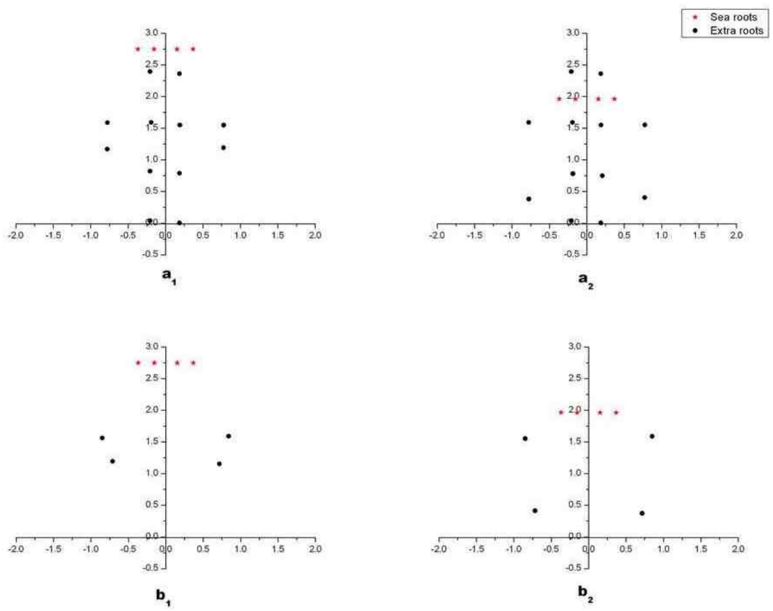

Figure 5.4: Ground-state Bethe roots for $p = 3$, $N = 4$, $\alpha_- = 1.554i$, $\alpha_+ = 0.948i$, $\beta_- = -0.214$, $\beta_+ = 0.186$, $\theta_- = 0.6i$, $\theta_+ = 0.7i$.

functions:

$$\begin{aligned} w_k^{\pm(b_j)} &= \pm\tilde{w}_k + (p-k)\,\eta\,, \qquad k = 1\,,\ldots\,,p-2\,, \\ w_{p-1}^{\pm(b_j)} &= \pm\tilde{w}_{p-1} + \left(\frac{p+2-2j}{2}\right)\eta\,, \qquad j = 1\,,\ldots\,,\frac{p+1}{2}\,. \end{aligned} \tag{5.46}$$

Similarly to the even p case, the real parts of the extra roots are related to each other pairwise,

$$\tilde{w}_k = \tilde{w}_{p-k-1}\,, \qquad k = 1\,,\ldots\,,\frac{p-3}{2}\,, \tag{5.47}$$

so that only $\tilde{w}_{\frac{p-1}{2}}$ remains unpaired.

Similarly, the extra roots of the $a_j(u)$ functions are as follows,

$$\begin{aligned} w_k^{\pm(a_j,1)} &= w_k^{\pm(b_j)} = \pm\tilde{w}_k + (p-k)\,\eta\,, \quad k = 1\,,\ldots\,,p-2\,, \\ w_{p-1}^{\pm(a_j,1)} &= w_{p-1}^{\pm(b_j)} = \pm\tilde{w}_{p-1} + \left(\frac{p+2-2j}{2}\right)\eta\,, \end{aligned}$$

$$w_k^{\pm(a_j,2)} = \pm\tilde{w}_0 + (p+1-k)\,\eta\,, \quad k = 1\,, \ldots\,, p+1\,, \qquad j = 1\,, \ldots\,, \frac{p+1}{2}\,. \tag{5.48}$$

As in the even p case, the extra roots of the first type $\{w_k^{\pm(a_j,1)}\}$ coincide with the b roots $\{w_k^{\pm(b_j)}\}$. Moreover, the extra roots of the second type $\{w_k^{\pm(a_j,2)}\}$ form a "$(p+1)$-string", with real part $\tilde{w}_0$.

However, in contrast to the even p case, some of the extra roots (namely, $w_{p-1}^{(a_j,1)}$ and $w_{p-1}^{(b_j)}$) depend on the value of j. Hence, as we shall see, these extra roots will not cancel from either the energy expression or the Bethe equations. Nevertheless, the contribution of these roots to the boundary energy will ultimately cancel.

5.3.3 Boundary energy

As in the case of even p, we use the energy expression (5.19) and the string hypothesis to obtain (for $p \ge 3$)

$$\begin{aligned} E &= \frac{1}{2}\sinh\eta\Bigg\{\sum_{k=1}^{\frac{N}{2}}\Big[\coth(v_k^{+(b_j)} + (j-1)\eta) + \coth(v_k^{-(b_j)} + (j-1)\eta) \\ &- \coth(v_k^{+(b_{j-1})} + (j-1)\eta) - \coth(v_k^{-(b_{j-1})} + (j-1)\eta)\Big] \\ &+ \sum_{k=1}^{p-1}\Big[\coth(w_k^{+(b_j)} + (j-1)\eta) + \coth(w_k^{-(b_j)} + (j-1)\eta) \\ &- \coth(w_k^{+(b_{j-1})} + (j-1)\eta) - \coth(w_k^{-(b_{j-1})} + (j-1)\eta)\Big]\Bigg\} + E_0\,, \\ &\qquad j = 2\,, \ldots\,, \frac{p+1}{2}\,. \end{aligned} \tag{5.49}$$

Recalling (5.45) and (5.46), this expression for the energy reduces, independently of the value of j, to

$$E = \sinh^2\eta\sum_{k=1}^{\frac{N}{2}}\frac{1}{\sinh(\tilde{v}_k - \frac{\eta}{2})\sinh(\tilde{v}_k + \frac{\eta}{2})} - \frac{2\sinh^2\eta}{\cosh\eta + \cosh(2\tilde{w}_{p-1})} + E_0\,, \tag{5.50}$$

where $\tilde{v}_k\,, \tilde{w}_{p-1} > 0$. As already anticipated, the expression for the energy depends on the extra root $\tilde{w}_{p-1}$ as well as on the sea roots.

Turning now to the Bethe Ansatz equations, following similar arguments as for the even p case, we find again that the A normalization constants are all equal, and similarly for the B's,

$$A_1 = A_2 = \ldots = A_{\frac{p+1}{2}}\,, \qquad B_1 = B_2 = \ldots = B_{\frac{p+1}{2}}\,. \tag{5.51}$$

Choosing $u_l^{(b_j)}$ in (5.9) to be a sea root $v_l^{+(b_j)}$ for any $j \in \{2\,, \ldots\,, \frac{p+1}{2}\}$, we obtain

$$\begin{aligned}
&\left(\frac{\sinh(\tilde{v}_l + \frac{\eta}{2})}{\sinh(\tilde{v}_l - \frac{\eta}{2})}\right)^{2N} \frac{\sinh(2\tilde{v}_l + \eta)}{\sinh(2\tilde{v}_l - \eta)} \frac{\sinh(\tilde{v}_l - \frac{\eta}{2} + \alpha_-)}{\sinh(\tilde{v}_l + \frac{\eta}{2} - \alpha_-)} \frac{\cosh(\tilde{v}_l - \frac{\eta}{2} + \beta_-)}{\cosh(\tilde{v}_l + \frac{\eta}{2} - \beta_-)} \\
&\quad\times \frac{\sinh(\tilde{v}_l - \frac{\eta}{2} + \alpha_+)}{\sinh(\tilde{v}_l + \frac{\eta}{2} - \alpha_+)} \frac{\cosh(\tilde{v}_l - \frac{\eta}{2} + \beta_+)}{\cosh(\tilde{v}_l + \frac{\eta}{2} - \beta_+)} = -\frac{\sinh(\tilde{v}_l - \tilde{w}_{p-1} - \frac{p-1}{2}\eta)}{\sinh(\tilde{v}_l - \tilde{w}_{p-1} + \frac{p-1}{2}\eta)} \\
&\quad\times \frac{\sinh(\tilde{v}_l + \tilde{w}_{p-1} - \frac{p-1}{2}\eta)}{\sinh(\tilde{v}_l + \tilde{w}_{p-1} + \frac{p-1}{2}\eta)} \prod_{k=1}^{\frac{N}{2}} \frac{\sinh(\tilde{v}_l - \tilde{v}_k + \eta)}{\sinh(\tilde{v}_l - \tilde{v}_k - \eta)} \frac{\sinh(\tilde{v}_l + \tilde{v}_k + \eta)}{\sinh(\tilde{v}_l + \tilde{v}_k - \eta)}\,, \\
&\quad l = 1\,, \cdots\,, \frac{N}{2}\,, \quad \tilde{v}_k\,, \tilde{w}_{p-1} > 0\,.
\end{aligned} \tag{5.52}$$

In a compact form, this result can be written as

$$\begin{aligned}
e_1(\lambda_l)^{2N+1}\, g_1(\lambda_l) \frac{e_{2a_- -1}(\lambda_l)\ e_{2a_+ -1}(\lambda_l)}{g_{1+2ib_-}(\lambda_l)\ g_{1+2ib_+}(\lambda_l)} &= -\Big[e_{p-1}(\lambda_l - \bar{\lambda})\ e_{p-1}(\lambda_l + \bar{\lambda})\Big]^{-1} \\
&\times \prod_{k=1}^{\frac{N}{2}} e_2(\lambda_l - \lambda_k)\ e_2(\lambda_l + \lambda_k)\,, \qquad l = 1\,, \cdots\,, \frac{N}{2}\,,
\end{aligned} \tag{5.53}$$

where $\tilde{w}_{p-1} = \mu\bar{\lambda}$. The corresponding ground state counting function is given by

$$\begin{aligned}
\mathsf{h}(\lambda) &= \frac{1}{2\pi}\Big\{(2N+1)q_1(\lambda) + r_1(\lambda) + q_{2a_- -1}(\lambda) - r_{1+2ib_-}(\lambda) + q_{2a_+ -1}(\lambda) \\
&- r_{1+2ib_+}(\lambda) + q_{p-1}(\lambda - \bar{\lambda}) + q_{p-1}(\lambda + \bar{\lambda}) \\
&- \sum_{k=1}^{\frac{N}{2}} \left[q_2(\lambda - \lambda_k) + q_2(\lambda + \lambda_k)\right]\Big\}\,.
\end{aligned} \tag{5.54}$$

Following similar procedure as before, we arrive at the root density for the ground state

$$\rho(\lambda) = 2a_1(\lambda) - \int_{-\infty}^{\infty} d\lambda'\ a_2(\lambda - \lambda')\ \rho(\lambda') + \frac{1}{N}\Big[a_1(\lambda) + b_1(\lambda) + a_2(\lambda) \tag{5.55}$$

$$
\begin{aligned}
&+ \quad a_{2a_- -1}(\lambda) - b_{1+2ib_-}(\lambda) + a_{2a_+ -1}(\lambda) - b_{1+2ib_+}(\lambda) + a_{p-1}(\lambda - \bar{\lambda}) \\
&+ \quad a_{p-1}(\lambda + \bar{\lambda})\Big] \,,
\end{aligned}
$$

where as before higher order corrections in $1/N$ are ignored when passing from a sum to an integral. This yields

$$
\rho(\lambda) = 2s(\lambda) + \frac{1}{N} R(\lambda) \,, \tag{5.56}
$$

where now

$$
\begin{aligned}
\hat{R}(\omega) \quad &= \quad \frac{1}{(1 + \hat{a}_2(\omega))} \Big\{ \hat{a}_1(\omega) + \hat{b}_1(\omega) + \hat{a}_2(\omega) - \hat{b}_{1+2ib_-}(\omega) - \hat{b}_{1+2ib_+}(\omega) \\
&+ \quad \hat{a}_{2a_- -1}(\omega) + \hat{a}_{2a_+ -1}(\omega) + 2\cos(\bar{\lambda}\omega)\, \hat{a}_{p-1}(\omega) \Big\} \,.
\end{aligned} \tag{5.57}
$$

The energy expression (5.50) yields, as $N \to \infty$,

$$
\begin{aligned}
E \quad &= \quad -\frac{2\pi \sin \mu}{\mu} \Big\{ \sum_{k=1}^{\frac{N}{2}} a_1(\lambda_k) + b_1(\bar{\lambda}) \Big\} + E_0 \\
&= \quad -\frac{\pi \sin \mu}{\mu} \Big\{ \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} a_1(\lambda_k) - a_1(0) + 2b_1(\bar{\lambda}) \Big\} + E_0 \\
&= \quad -\frac{\pi \sin \mu}{\mu} \Big\{ N \int_{-\infty}^{\infty} d\lambda \ a_1(\lambda) \ \rho(\lambda) - a_1(0) + 2b_1(\bar{\lambda}) \Big\} + \frac{1}{2}(N-1)\cos\mu \\
&+ \quad \frac{1}{2} \sin\mu \left(\cot \mu a_- + i \tanh \mu b_- + \cot \mu a_+ + i \tanh \mu b_+ \right) \,.
\end{aligned} \tag{5.58}
$$

Substituting (5.56) for the root density, we again obtain

$$
E = E_{bulk} + E_{boundary} \,, \tag{5.59}
$$

where the bulk (order N) energy is again given by (5.41). The boundary energy is now given by

$$
\begin{aligned}
E_{boundary} \quad &= \quad -\frac{\pi \sin \mu}{\mu} I + \frac{1}{2} \sin\mu \left(\cot \mu a_- + i \tanh \mu b_- + \cot \mu a_+ + i \tanh \mu b_+ \right) \\
&- \quad \frac{2\pi \sin \mu}{\mu} b_1(\bar{\lambda}) - \frac{1}{2} \cos \mu \,,
\end{aligned} \tag{5.60}
$$

where I is now the integral

$$\begin{aligned} I &= \int_{-\infty}^{\infty} d\lambda\ a_1(\lambda)\left[R(\lambda)-\delta(\lambda)\right] = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\ \hat{a}_1(\omega)\left[\hat{R}(\omega)-1\right] \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\ \hat{s}(\omega)\Big\{\hat{a}_1(\omega)+\hat{b}_1(\omega)-1 \\ &\quad -\hat{b}_{1+2ib_-}(\omega)-\hat{b}_{1+2ib_+}(\omega)+\hat{a}_{2a_--1}(\omega)+\hat{a}_{2a_+-1}(\omega)+2\cos(\bar{\lambda}\omega)\,\hat{a}_{p-1}(\omega)\Big\}\,. \end{aligned} \tag{5.61}$$

Using the fact that $\hat{s}(\omega)\hat{a}_{p-1}(\omega) = -\hat{b}_1(\omega)$, we see that there is a perfect cancellation of the last term in (5.60) which depends on the extra root $\bar{\lambda}$. Thus, as in the even p case, there is no contribution to the boundary energy from extra roots. Proceeding as before, we find that the energy contribution from each boundary is again given by (5.44), thus coinciding with previous results, (4.4) and (4.66).

As for even p, the derivation here is based on the string hypothesis for the ground-state Bethe roots, which is true only for suitable values of boundary parameters. For example, the shaded areas in Figures 5.5 and 5.6 denote the regions of parameter space for which the ground-state Bethe roots have the form described in Sections 5.3.1 and 5.3.2. The $\alpha_\pm$ and $\beta_\pm$ parameters are varied in the two figures, respectively.

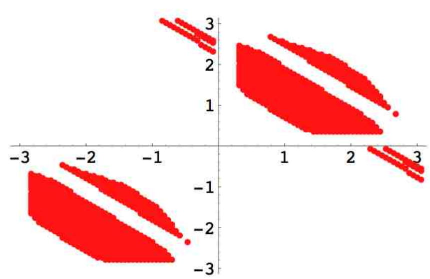

Figure 5.5: Shaded area denotes region of the $(\Im m\,\alpha_+\,,\Im m\,\alpha_-)$ plane for which the ground-state Bethe roots obey the string hypothesis for $p=3$, $N=2$, $\beta_-=-0.85$, $\beta_+=0.9$, $\theta_-=0.6i$, $\theta_+=0.7i$.

We have studied the ground state of the general integrable open XXZ spin-1/2 chain (2.1) in the thermodynamic limit, utilizing the solution we found recently

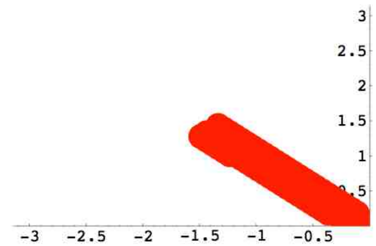

Figure 5.6: Shaded area denotes region of the $(\beta_+\,,\beta_-)$ plane for which the ground-state Bethe roots obey the string hypothesis for $p = 3$, $N = 2$, $\alpha_- = 1.2i$, $\alpha_+ = 0.98i$, $\theta_- = 0.7i$, $\theta_+ = 0.6i$.

in [60] which does not assume any restrictions or constraints among the boundary parameters. However, the bulk parameter is restricted to values corresponding to roots of unity. The key to working with this solution is formulating an appropriate string hypothesis, which leads to a reduction of the Bethe Ansatz equations to a conventional form. While the idea of using a string hypothesis to simplify the analysis of Bethe equations is as old as the Bethe Ansatz itself, the particular patterns appearing here are perhaps unparalleled in their rich structure.

The boundary energy result (5.44) was obtained previously [42] for bulk and boundary parameters that are unconstrained and constrained, respectively; and we have now obtained the same result for the reversed situation, namely, for bulk and boundary parameters that are constrained and unconstrained, respectively. Hence, this result presumably holds when both the bulk and boundary parameters are unconstrained (within some suitable domains). Indeed, for the boundary sine-Gordon model [6], which is closely related to the open XXZ chain, the expression [59] for the boundary energy is valid for general values of the bulk and boundary parameters.

Having demonstrated the practicality of this solution, we now expect that it should be possible to use a similar approach to analyze further properties of the model, such as the Casimir energy (order $1/N$ correction to the ground state energy), and bulk and boundary excited states.

There is an evident redundancy in the solution which we have used here: there are many equivalent expressions for the energy (see, e.g., (5.19), (5.21)), and we find that the Bethe Ansatz equations (5.7), (5.9) all become equivalent upon imposing the string hypothesis. Moreover, while there are various “extra” Bethe roots describing the ground state, they ultimately do not contribute to the boundary energy. All of this suggests that it may be possible to find a simpler and more economical solution of the model involving fewer Q functions. Ideally, one would like to find a solution for which neither bulk nor boundary parameters are constrained.

Chapter 6: Finite-Size Correction and Bulk Hole-Excitations

The integrable open spin-1/2 XXZ chain has been subjected to intensive studies due to its growing applications in various fields of physics, e.g., statistical mechanics, string theory and condensed matter physics. Various progress have been made in obtaining solutions for this model, both diagonal [14, 15, 23] and general nondiagonal cases [24], [26]–[31]. Upon obtaining the desired solution, the next natural question that needed to be addresed is its practicality within various contexts. One important area where these solutions have found creditable applications is in determining finite size corrections to the ground state energy. By relating to conformal invariance, these finite size corrections are shown to be related directly to other crucial parameters like the critical indices, central charge and conformal dimensions [62]–[65]. There are few methods and approaches to accomplish this task. De Vega and Woynarowich [66] derived integral equations for calculating leading finite-size corrections for models solvable by Bethe Ansatz approach [67]. This was then generalized to nested Bethe Ansatz models as well [68]. Another approach was introduced by Woynarowich and Eckel [69, 70], which utilizes Euler-Maclaurin formula and Wiener-Hopf integration to compute these corrections for the closed XXZ chain. Others have also studied more general integrable spin chain models e.g., XXZ diagonal [15, 57], nondiagonal cases [42], quantum spin 1/2 chains with non-nearest-neighbour short-range interaction [71] and $XXZ(1/2, 1)$ which contains alternating spins of 1/2 and 1 [72], within similar framework. Other approaches e.g., based on NLIE (Nonlinear Integral Equations) have also been successful in determining these effects for integrable lattice models [73] and related integrable quantum field theories, such as the sine-Gordon model with periodic [74]–[77], Dirichlet [78]–[82] and Neumann boundary conditions [42, 43].

With similar aim in mind, utilizing an exact solution for the integrable spin-1/2 XXZ chain with nondiagonal boundary terms we found earlier for even number of sites [52, 53], and extending the solution to account for odd number of sites as well, we compute the correction of order $1/N$ (Casimir energy) to the ground state energy together with its low lying excited states (multi-hole states). We employ the method introduced by Woynarovich and Eckle [69] that makes use of Euler-Maclaurin formula [86] and Wiener-Hopf integration [87]. In particular, we compute the analytical expressions for central charge and the conformal dimensions of low lying excited states. We also compare these analytical results to corresponding numerical results obtained by solving the model numerically for some large number of sites.

Bethe Ansatz solution will be reviewed and extension of that result to include the corresponding Bethe Ansatz solution for odd N makes our final result more complete. We notice that the lowest energy state for even N of this model has one hole. Hence, the true ground state (lowest energy state without holes) lies in the odd N sector. Similar behaviour are also found for the open chain with diagonal boundary terms, for certain values of boundary parameters [88]. It is known that (critical) XXZ model with nondiagonal boundary terms corresponds to (conformally invariant) free Boson with Neumann boundary condition whereas the diagonal ones are related to the Dirichlet case [43, 79, 80, 81]. Although the model we study here has nondiagonal boundary terms, we find that the conformal dimensions for this model resemble that of the Dirichlet boundary condition. Numerical results are presented to confirm and support the analytical results. Here, we solve the model numerically for some large but finite N and further employ an algorithm due to Vanden Broeck and Schwartz [83, 84] to extrapolate the results for $N \to \infty$ limit.

6.1 Bethe Ansatz

We begin this section by reviewing the Bethe Ansatz solution for the model (4.41). Note that, this model has only two boundary parameters. Other boundary parameters (as they appear in the original Hamiltonian in (2.1)) have been set to zero. We restrict the values of $\alpha_\pm$ to be pure imaginary to ensure the Hermiticity of the Hamiltonian. The Bethe Ansatz equations for both odd and even N are given by

$$\begin{aligned}
\frac{\delta(u_j^{(1)})\ h^{(2)}(u_j^{(1)}-\eta)}{\delta(u_j^{(1)}-\eta)\ h^{(1)}(u_j^{(1)})} &= -\frac{Q_2(u_j^{(1)}-\eta)}{Q_2(u_j^{(1)}+\eta)}\,, \qquad j = 1\,,2\,,\ldots\,,M_1\,, \\
\frac{h^{(1)}(u_j^{(2)}-\eta)}{h^{(2)}(u_j^{(2)})} &= -\frac{Q_1(u_j^{(2)}+\eta)}{Q_1(u_j^{(2)}-\eta)}\,, \qquad j = 1\,,2\,,\ldots\,,M_2\,.
\end{aligned} \tag{6.1}$$

where $\delta(u)$ is given by (2.17), (2.18) and (2.19). $Q_a(u)$ is given by (4.44). However, $h^{(1)}(u)$ and $h^{(2)}(u)$ differ for odd and even values of N. The energy eigenvalues in terms of the "shifted" Bethe roots $\tilde{u}_j^{(a)}$ are given by

$$E = \frac{1}{2}\sinh^2\eta\sum_{a=1}^{2}\sum_{j=1}^{M_a}\frac{1}{\sinh(\tilde{u}_j^{(a)}-\frac{\eta}{2})\sinh(\tilde{u}_j^{(a)}+\frac{\eta}{2})} + \frac{1}{2}(N-1)\cosh\eta\,. \tag{6.2}$$

where $\tilde{u}_j^{(a)} \equiv u_j^{(a)} + \frac{\eta}{2}$.

6.1.1 Even N

The Bethe roots $\tilde{u}_j^{(a)}$ for the lowest energy state have the form (4.51). The Bethe Ansatz equations for the sea roots are given by (4.53) and (4.54) respectively, where $j = 1\,,\ldots\,,\frac{N}{2}$. The corresponding ground-state counting functions are given by (4.55) and (4.56) respectively. These counting functions satisfy the following

$$\mathsf{h}^{(l)}(\lambda_j) = j\,, \qquad j = 1\,,\ldots\,,\frac{N}{2} \tag{6.3}$$

In (6.3) above, $l = 1\,,2$.

6.1.2 Odd N

In this section, we present an extension of the previous results to include solutions for odd N values. The roots distribution is similar to the previous case, but now we have $M_{(1,1)} = M_{(2,1)} = \frac{N+1}{2}$, and $M_{(1,2)} = M_{(2,2)} = \frac{p-1}{2}$. Using the following in (6.1),

$$\begin{aligned} h^{(1)}(u) &= \sinh(u-\alpha_+ +\eta)\sinh(u+\alpha_+ +\eta) \\ &\times \frac{\sinh^{2N+1}(u+2\eta)\cosh^2(u+\eta)\cosh(u+2\eta)}{\sinh(2u+3\eta)}, \\ & h^{(2)}(u) = h^{(1)}(-u-2\eta)\,, \end{aligned} \tag{6.4}$$

we obtain the Bethe Ansatz equations

$$\begin{aligned} & e_1(\lambda_j^{(1,1)})^{2N+1}\left[g_1(\lambda_j^{(1,1)})e_{1+2a_-}(\lambda_j^{(1,1)})e_{1-2a_-}(\lambda_j^{(1,1)})\right]^{-1} \\ &= -\prod_{k=1}^{(N+1)/2}\left[e_2(\lambda_j^{(1,1)}-\lambda_k^{(2,1)})e_2(\lambda_j^{(1,1)}+\lambda_k^{(2,1)})\right] \\ &\times \prod_{k=1}^{(p-1)/2}\left[g_2(\lambda_j^{(1,1)}-\lambda_k^{(2,2)})g_2(\lambda_j^{(1,1)}+\lambda_k^{(2,2)})\right], \end{aligned} \tag{6.5}$$

and

$$\begin{aligned} & e_1(\lambda_j^{(2,1)})^{2N+1}\left[g_1(\lambda_j^{(2,1)})e_{1+2a_+}(\lambda_j^{(2,1)})e_{1-2a_+}(\lambda_j^{(2,1)})\right]^{-1} \\ &= -\prod_{k=1}^{(N+1)/2}\left[e_2(\lambda_j^{(2,1)}-\lambda_k^{(1,1)})e_2(\lambda_j^{(2,1)}+\lambda_k^{(1,1)})\right] \\ &\times \prod_{k=1}^{(p-1)/2}\left[g_2(\lambda_j^{(2,1)}-\lambda_k^{(1,2)})g_2(\lambda_j^{(2,1)}+\lambda_k^{(1,2)})\right], \end{aligned} \tag{6.6}$$

respectively, where $j = 1, \ldots, \frac{N+1}{2}$. Note the presence of parameter-dependant terms in both the equations above. One can also notice the number of extra roots changes from $\frac{p+1}{2}$ to $\frac{p-1}{2}$ for $Q_1(u)$. The ground-state counting functions for this case read

$$\mathsf{h}^{(1)}(\lambda) = \frac{1}{2\pi}\Big\{(2N+1)q_1(\lambda) - r_1(\lambda) - q_{1+2a_-}(\lambda) - q_{1-2a_-}(\lambda)$$

$$- \sum_{k=1}^{(N+1)/2} \left[q_2(\lambda - \lambda_k^{(2,1)}) + q_2(\lambda + \lambda_k^{(2,1)}) \right] - \sum_{k=1}^{(p-1)/2} \left[r_2(\lambda - \lambda_k^{(2,2)}) + r_2(\lambda + \lambda_k^{(2,2)}) \right] \Big\} , \tag{6.7}$$

and

$$\mathsf{h}^{(2)}(\lambda) = \frac{1}{2\pi} \Big\{ (2N+1) q_1(\lambda) - r_1(\lambda) - q_{1+2a_+}(\lambda) - q_{1-2a_+}(\lambda)$$
$$- \sum_{k=1}^{(N+1)/2} \left[q_2(\lambda - \lambda_k^{(1,1)}) + q_2(\lambda + \lambda_k^{(1,1)}) \right] - \sum_{k=1}^{(p-1)/2} \left[r_2(\lambda - \lambda_k^{(1,2)}) + r_2(\lambda + \lambda_k^{(1,2)}) \right] \Big\} , \tag{6.8}$$

As for even N, we again have the following

$$\mathsf{h}^{(l)}(\lambda_j) = j \,, \qquad j = 1 \,, \ldots \,, \frac{N+1}{2} \tag{6.9}$$

where $l = 1\,,2$. Note that (6.3) and (6.9) can be written more compactly as

$$\mathsf{h}^{(l)}(\lambda_j) = j \,, \qquad j = 1 \,, \ldots \,, \lfloor \frac{N+1}{2} \rfloor \tag{6.10}$$

where $\lfloor \ldots \rfloor$ denotes the integer part and $\mu \lambda_{\lfloor \frac{N+1}{2} \rfloor}$ is the largest sea root for that "sea." Subsequently, we shall denote largest sea roots as $\mu \Lambda_l$.

6.2 Finite-size correction of order $1/N$

In this section, we shall compute the finite-size correction for the ground state and low lying excited states. For these excited states, we restrict our analysis to excitations by holes which are located to the right of the real sea roots. Applying (4.51) to (6.2), we get the lowest state energy eigenvalues for chain of finite length N,

$$E = -\frac{\pi \sin \mu}{\mu} \Big\{ \frac{1}{2} \sum_{a=1}^{2} \sum_{j=-\lfloor \frac{N+1}{2} \rfloor}^{\lfloor \frac{N+1}{2} \rfloor} a_1(\lambda_j^{(a,1)}) - a_1(0) + \sum_{a=1}^{2} \sum_{j=1}^{M_{(a,2)}} b_1(\lambda_j^{(a,2)}) \Big\}$$
$$+ \frac{1}{2}(N-1) \cos \mu \,. \tag{6.11}$$

where earlier notations for $a_n(\lambda)$ and $b_n(\lambda)$ have again been adopted. Note that $M_{(a,2)}$ in (6.11), refers to number of extra roots for $Q_a(u)$. The first and third terms in the curly bracket of (6.11) are summed over the number of sea roots and extra roots respectively. As one considers next lowest excited state, the number of sea roots and extra roots change. Hence, for these states of low lying excitations (with real sea), the very same term in the first sum will again be summed over accordingly between approriate limits dictated by the number of sea roots. As for the summation over extra roots, the function summed over depends on the imaginary part of these roots, especially in the presence of 2-strings. However, as one shall see, for $1/N$ correction (in the $N \to \infty$ limit), only the sum over the sea roots contributes. The second sum in (6.11) contributes to order 1 correction (boundary energy) which we have considered in Chapter 4 [25].

6.2.1 Sum-rule and hole-excitations

Now we present some results based on the solution of the model (4.41) for $N = 2\,,3\,,\ldots\,,7$. We begin with even N case. We find for even N, excited states contain odd number of holes for each $Q_a(u)$. This can be seen from the following analysis on counting functions. For the lowest energy state the counting functions are given by (4.55) and (4.56). By using the fact that $q_n(\lambda) \to \mathrm{sgn}(n)\pi - \mu n$ and $r_n(\lambda) \to -\mu n$ as $\lambda \to \infty$ and $\rho^{(l)} = \frac{1}{N}\frac{d\mathsf{h}^{(l)}}{d\lambda}$ we have the following sum rule

$$\begin{aligned} \int_{\Lambda_l}^{\infty} d\lambda\, \rho^{(l)}(\lambda) &= \frac{1}{N}(\mathsf{h}^{(l)}(\infty) - \mathsf{h}^{(l)}(\Lambda_l)) \\ &= \frac{1}{N}(\frac{1}{2} + 1) \end{aligned} \tag{6.12}$$

$\mu\Lambda_l$ refers to the largest sea root. As before $l = 1\,,2$. We make use of the fact that

$$\begin{aligned} \mathsf{h}^{(l)}(\infty) &= \frac{N}{2} + \frac{3}{2} \\ \mathsf{h}^{(l)}(\Lambda_l) &= \frac{N}{2} \end{aligned} \tag{6.13}$$

[25] Equation (4.66) for the boundary energy holds both for even and odd values of N

From (6.12) and (6.13), we see that there is one hole located to the right of the largest sea root. Similar analysis for low lying (multi-hole) excited states yields the following

$$\begin{aligned} \int_{\Lambda_l}^{\infty} d\lambda\; \rho^{(l)}(\lambda) &= \frac{1}{N}(\mathsf{h}^{(l)}(\infty) - \mathsf{h}^{(l)}(\Lambda_l)) \\ &= \frac{1}{N}(\frac{1}{2} + N_H) \end{aligned} \tag{6.14}$$

where N_H is the number of holes (odd) to the right of the corresponding largest sea root. To illustrate the results above, we consider the following low lying excited states with $\frac{N}{2}-1$ and $\frac{N}{2}-2$ sea roots and therefore different number of extra roots than the lowest energy state [26]. The former case is found to have one hole with $\frac{p-1}{2}$ and $\frac{p-3}{2}$ extra roots in addition to a 2-string from each of the $Q_1(u)$ and $Q_2(u)$ respectively. From,

$$\begin{aligned} \mathsf{h}^{(l)}(\infty) = \frac{N}{2} + \frac{1}{2} \\ \mathsf{h}^{(l)}(\Lambda_l) = \frac{N}{2} - 1 \end{aligned} \tag{6.15}$$

one has

$$\frac{1}{N}(\mathsf{h}^{(l)}(\infty) - \mathsf{h}^{(l)}(\Lambda_l)) = \frac{1}{N}(\frac{1}{2} + 1) \tag{6.16}$$

Hence giving $N_H = 1$. The later case has three holes with $\frac{p+1}{2}$ and $\frac{p-1}{2}$ extra roots and a 2-string from each of the $Q_a(u)$ with $a = 1\,, 2$. Similar analysis,

$$\begin{aligned} \mathsf{h}^{(l)}(\infty) = \frac{N}{2} + \frac{3}{2} \\ \mathsf{h}^{(l)}(\Lambda_l) = \frac{N}{2} - 2 \end{aligned} \tag{6.17}$$

yields

$$\frac{1}{N}(\mathsf{h}^{(l)}(\infty) - \mathsf{h}^{(l)}(\Lambda_l)) = \frac{1}{N}(\frac{1}{2} + 3) \tag{6.18}$$

[26] The lowest energy state has $\frac{N}{2}$ sea roots. As for the extra roots, there are $\frac{p+1}{2}$ and $\frac{p-1}{2}$ of them for $Q_1(u)$ and $Q_2(u)$ respectively

giving $N_H = 3$. The total number of roots are the same for all these states. There are also excited states with equal number of sea and extra roots as for the state of lowest energy, but with position of the single hole nearer to the origin than that of the lowest energy state, suggesting the usual bulk hole-excitation scenario, $E_{hole}(\lambda^{(a)})$ increases as $\lambda^{(a)} \to 0$ where $E_{hole}(\lambda^{(a)})$ is the energy due to the presence of holes and $\lambda^{(a)}$, with $a = 1\,,2$ denote the positions of the holes in both "seas." We shall compute the explicit expression for energy due to holes shortly.

As for the odd N case, we have the true ground state, namely state of lowest energy without hole. From the counting functions, (6.7) and (6.8), we have

$$\begin{aligned} \int_{\Lambda_l}^{\infty} d\lambda\ \rho^{(l)}(\lambda) &= \frac{1}{N}(\mathsf{h}^{(l)}(\infty) - \mathsf{h}^{(l)}(\Lambda_l)) \\ &= \frac{1}{2N} \end{aligned} \tag{6.19}$$

As before $l = 1\,,2$, and we make use of the fact that

$$\begin{aligned} \mathsf{h}^{(l)}(\infty) &= \frac{N}{2} + 1 \\ \mathsf{h}^{(l)}(\Lambda_l) &= \frac{N+1}{2} \end{aligned} \tag{6.20}$$

From (6.20), we see that this state of lowest energy for odd N has no hole, signifying the true ground state. Similar analysis for low lying excited states yields the following

$$\begin{aligned} \int_{\Lambda_l}^{\infty} d\lambda\ \rho^{(l)}(\lambda) &= \frac{1}{N}(\mathsf{h}^{(l)}(\infty) - \mathsf{h}^{(l)}(\Lambda_l)) \\ &= \frac{1}{N}(\frac{1}{2} + N_H) \end{aligned} \tag{6.21}$$

where N_H is the number of holes (even) to the right of sea roots. Hence, for odd N case, there are even number of holes (for each $Q_a(u)$), with $a = 1\,,2$, for the excited states, e.g., for the first excited state with $\frac{N-1}{2}$ sea roots,

$$\begin{aligned} \mathsf{h}^{(l)}(\infty) &= \frac{N+1}{2} + \frac{3}{2} \\ \mathsf{h}^{(l)}(\Lambda_l) &= \frac{N-1}{2} \end{aligned} \tag{6.22}$$

which signifies the presence of two holes.

It is known for simpler models of spin chains e.g., closed XXZ chain that even number of holes are present in chains with even number of spins and vice versa. Hence, the true ground state (lowest energy state with no holes) for these models is found to lie in even N sector. The reverse scenario (one hole in the lowest energy state for even N and ground state in odd N sector) we find here for this model can be explained using some heuristic arguments based on spin and magnetic fields at the two boundaries, similar to the one given at the end of Section 4.1 [27]. From (4.67), we notice the signs of a_+ and a_- must be the same for boundary parameter region of interest. Hence, in Hamiltonian (4.41), the direction of the magnetic fields at the two boundaries are also the same (Both up or both down). This upsets the antiferromagnetic spin arrangement at the boundaries, favouring spin allignments along the same direction at the boundaries for chains with even N. This causes the following: presence of odd N behaviours in the even N chain, namely the lowest energy state for even N sector has one hole for each $Q_a(u)$. Spins at the boundaries for the odd N chain will not experience such spin upset since the parallel magnetic fields favours the antiferromagnetic arrangement of an odd N chain. Therefore, the lowest energy state for odd N chain has no holes. In other words, the true ground state exists in odd N sector. Further effects are the presence of odd and even number of holes in chains with even and odd N respectively as shown in the analysis above.

Now, the energy due to hole excitations can be presented. We consider first the lowest energy state for even N case with one hole. Using

$$\frac{1}{N}\sum_{k=-\frac{N}{2}}^{\frac{N}{2}} g(\lambda - \lambda_k^{(a,1)}) \approx \int_{-\infty}^{\infty} d\lambda'\ \rho^{(l)}(\lambda') g(\lambda - \lambda') - \frac{1}{N} g(\lambda - \tilde{\lambda}^{(a)}) \tag{6.23}$$

[27] Readers are urged to refer to Figures 4.2 and 4.3.

for some arbitrary function $g(\lambda)$ and

$$\rho^{(l)} = \frac{1}{N}\frac{d\mathsf{h}^{(l)}}{d\lambda} \tag{6.24}$$

where $l = 1\,,2$, $\mu\lambda_k^{(a,1)} \equiv$ sea roots, with $a = 1\,,2$, and $\mu\tilde{\lambda}^{(a)} \equiv$ position of the hole for each of the $Q_a(u)$, one can write down the sum of the two densities

$$\begin{aligned}
\rho^{(1)}(\lambda) + \rho^{(2)}(\lambda) &= 4a_1(\lambda) - \int_{-\infty}^{\infty} d\lambda'\, (\rho^{(1)}(\lambda') + \rho^{(2)}(\lambda'))a_2(\lambda - \lambda') \\
&+ \frac{1}{N}[a_2(\lambda - \tilde{\lambda}^{(1)}) + a_2(\lambda - \tilde{\lambda}^{(2)})] + \frac{1}{N}[2a_1(\lambda) + 2a_2(\lambda) - 2b_1(\lambda) \\
&- a_{1+2a_-}(\lambda) - a_{1-2a_-}(\lambda) - a_{1+2a_+}(\lambda) - a_{1-2a_+}(\lambda) \\
&- \sum_{k=1}^{\frac{p-1}{2}}(b_2(\lambda - \lambda_k^{(2,2)}) + b_2(\lambda + \lambda_k^{(2,2)})) \\
&- \sum_{k=1}^{\frac{p+1}{2}}(b_2(\lambda - \lambda_k^{(1,2)}) + b_2(\lambda + \lambda_k^{(1,2)}))]
\end{aligned} \tag{6.25}$$

Defining $\rho_{total}(\lambda) \equiv \rho^{(1)}(\lambda) + \rho^{(2)}(\lambda)$ and solving (6.25) using Fourier transform, we have

$$\begin{aligned}
\hat{\rho}_{total}(\omega) &= 4\hat{s}(\omega) + \frac{1}{N}\hat{R}(\omega) \\
&+ \frac{1}{N}\hat{J}(\omega)(e^{i\omega\tilde{\lambda}^{(1)}} + e^{i\omega\tilde{\lambda}^{(2)}})
\end{aligned} \tag{6.26}$$

where $\hat{\rho}_{total}(\omega)\,, \hat{a}_2(\omega)$ and $\hat{s}(\omega)$ are the Fourier transforms of $\rho_{total(\lambda)}\,, a_2(\lambda)$ and $\frac{a_1(\lambda)}{1+a_2(\lambda)}$ respectively. Also $\hat{J}(\omega) = \frac{\hat{a}_2(\omega)}{1+\hat{a}_2(\omega)}$. $\hat{R}(\omega)$ is the contribution from the second square bracket in (6.25), which will not enter the calculation for $E_{hole}(\tilde{\lambda}^{(a)})$ and will be omitted henceforth. The Fourier transform of hole density are the third and the fourth terms in (6.26), which gives

$$\rho_{hole}(\lambda) = \frac{1}{N}[J(\lambda - \tilde{\lambda}^{(1)}) + J(\lambda - \tilde{\lambda}^{(2)})] \tag{6.27}$$

Using approximation (6.23) in (6.11), and making use of (6.27), one has

$$\begin{aligned}
E_{hole}(\tilde{\lambda}^{(a)}) &= -\frac{N\pi\sin\mu}{2\mu}\int_{-\infty}^{\infty} d\lambda\; a_1(\lambda)\rho_{hole}(\lambda) \\
&+ \frac{\pi\sin\mu}{2\mu}\sum_{a=1}^{2} a_1(\tilde{\lambda}^{(a)})
\end{aligned} \tag{6.28}$$

which after some manipulation yields

$$E_{hole}(\tilde{\lambda}^{(a)}) \quad = \quad \frac{\pi \sin\mu}{4\mu} \sum_{a=1}^{2} \frac{1}{\cosh \pi \tilde{\lambda}^{(a)}} \tag{6.29}$$

Generalizing the derivation to α number of holes, one has

$$\rho_{hole}(\lambda) = \frac{1}{N} \sum_{\alpha} \sum_{a=1}^{2} J(\lambda - \tilde{\lambda}_{\alpha}^{(a)}) \tag{6.30}$$

and finally the following for the energy

$$E_{hole}(\tilde{\lambda}_{\alpha}^{(a)}) \quad = \quad \frac{\pi \sin\mu}{4\mu} \sum_{\alpha} \sum_{a=1}^{2} \frac{1}{\cosh \pi \tilde{\lambda}_{\alpha}^{(a)}} \tag{6.31}$$

Note that $E_{hole}(\tilde{\lambda}_{\alpha}^{(a)})$ increases as $\tilde{\lambda}_{\alpha}^{(a)} \to 0$ as mentioned above in paragraph following (6.18).

6.2.2 Casimir energy

In this section, we give the derivation of $1/N$ correction (Casimir energy) to the lowest energy state, for the even N case (with one hole). This result is then generalized to include odd N values as well as the low lying (multi-hole) excited states. We begin by presenting the expression for the density difference between chain of finite length (with N spins), $\rho_N^{(1)}(\lambda) + \rho_N^{(2)}(\lambda)$ and that of infinite length, $\rho_\infty(\lambda)$

$$\begin{aligned}
\rho_N^{(1)}(\lambda) + \rho_N^{(2)}(\lambda) - \rho_\infty(\lambda) \quad &= \quad -\int_{-\infty}^{\infty} d\gamma \; a_2(\lambda - \gamma)[\frac{1}{N} \sum_{\beta=-\frac{N}{2}}^{\frac{N}{2}} \delta(\gamma - \lambda_\beta^{(1,1)}) - \rho_N^{(1)}(\gamma)] \\
&- \quad \int_{-\infty}^{\infty} d\gamma \; a_2(\lambda - \gamma)[\frac{1}{N} \sum_{\beta=-\frac{N}{2}}^{\frac{N}{2}} \delta(\gamma - \lambda_\beta^{(2,1)}) - \rho_N^{(2)}(\gamma)] \\
&- \quad \int_{-\infty}^{\infty} d\gamma \; a_2(\lambda - \gamma)[\rho_N^{(1)}(\gamma) + \rho_N^{(2)}(\gamma) - \rho_\infty(\gamma)]
\end{aligned} \tag{6.32}$$

In (6.32) and henceforth, only terms that are crucial to the computation of $1/N$ correction are given. Other parameter dependant terms that contribute to order 1 correction have been omitted here [28]. Solving (6.32) yields

$$\begin{aligned}\rho_N^{(1)}(\lambda)+\rho_N^{(2)}(\lambda)-\rho_\infty(\lambda) &= -\int_{-\infty}^{\infty}d\gamma\; p(\lambda-\gamma)[\frac{1}{N}\sum_{\beta=-\frac{N}{2}}^{\frac{N}{2}}\delta(\gamma-\lambda_\beta^{(1,1)})-\rho_N^{(1)}(\gamma)] \\ &- \int_{-\infty}^{\infty}d\gamma\; p(\lambda-\gamma)[\frac{1}{N}\sum_{\beta=-\frac{N}{2}}^{\frac{N}{2}}\delta(\gamma-\lambda_\beta^{(2,1)})-\rho_N^{(2)}(\gamma)]\end{aligned} \tag{6.33}$$

where $\rho_\infty(\lambda)=\frac{4a_1(\lambda)}{1+a_2(\lambda)}\equiv 4s(\lambda)$ and $p(\lambda)=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\; e^{-i\omega\lambda}\frac{\hat{a}_2(\omega)}{1+\hat{a}_2(\omega)}$ Similar equation expressing the energy difference between finite and infinite system is also needed to compute Casimir energy. This is given by

$$\begin{aligned}E_N-E_\infty &= -\frac{N\pi\sin\mu}{2\mu}\Big\{\int_{-\infty}^{\infty}d\lambda\; a_1(\lambda)[\frac{1}{N}\sum_{\beta=-\frac{N}{2}}^{\frac{N}{2}}\delta(\lambda-\lambda_\beta^{(1,1)})-\rho_N^{(1)}(\lambda)] \\ &+ \int_{-\infty}^{\infty}d\lambda\; a_1(\lambda)[\frac{1}{N}\sum_{\beta=-\frac{N}{2}}^{\frac{N}{2}}\delta(\lambda-\lambda_\beta^{(2,1)})-\rho_N^{(2)}(\lambda)] \\ &+ \int_{-\infty}^{\infty}d\lambda\; a_1(\lambda)[\rho_N^{(1)}(\lambda)+\rho_N^{(2)}(\lambda)-\rho_\infty(\lambda)]\Big\}\end{aligned} \tag{6.34}$$

Using (6.33) and the fact that $\hat{p}(\omega)\hat{a}_1(\omega)=\hat{s}(\omega)\hat{a}_2(\omega)$, we have

$$E_N-E_\infty = -\frac{N\pi\sin\mu}{4\mu}\Big\{\int_{-\infty}^{\infty}d\lambda\; S_N^{(1)}(\lambda)\rho_\infty^{(1)}(\lambda)+\int_{-\infty}^{\infty}d\lambda\; S_N^{(2)}(\lambda)\rho_\infty^{(2)}(\lambda)\Big\} \tag{6.35}$$

where $S_N^{(l)}(\lambda)\equiv\frac{1}{N}\sum_{\beta=-\frac{N}{2}}^{\frac{N}{2}}\delta(\lambda-\lambda_\beta^{(l,1)})-\rho_N^{(l)}(\lambda)$ and $\rho_\infty^{(l)}(\lambda)=\frac{1}{2}\rho_\infty(\lambda)\equiv 2s(\lambda)$ with $l=1\,,2$. Further, using Euler-Maclaurin summation formula [86], (6.35) becomes

$$\begin{aligned}E_N-E_\infty &= -\frac{N\pi\sin\mu}{2\mu}\Big\{-\int_{\Lambda_1}^{\infty}d\lambda\; \rho_\infty^{(1)}(\lambda)\rho_N^{(1)}(\lambda)+\frac{1}{2N}\rho_\infty^{(1)}(\Lambda_1) \\ &+ \frac{1}{12N^2\rho_N^{(1)}(\Lambda_1)}\rho_\infty^{(1)\prime}(\Lambda_1)-\int_{\Lambda_2}^{\infty}d\lambda\; \rho_\infty^{(2)}(\lambda)\rho_N^{(2)}(\lambda)+\frac{1}{2N}\rho_\infty^{(2)}(\Lambda_2) \\ &+ \frac{1}{12N^2\rho_N^{(2)}(\Lambda_2)}\rho_\infty^{(2)\prime}(\Lambda_2)\Big\}\end{aligned} \tag{6.36}$$

[28] See [53] for details

(6.33) can also be expressed in similar form

$$\begin{aligned}\rho_N^{(1)}(\lambda)+\rho_N^{(2)}(\lambda) &- \rho_\infty(\lambda)=\int_{\Lambda_1}^{\infty} d\gamma\ p(\lambda-\gamma)\rho_N^{(1)}(\gamma)-\frac{1}{2N}p(\lambda-\Lambda_1)\\ &- \frac{p^{'}(\lambda-\Lambda_1)}{12N^2\rho_N^{(1)}(\Lambda_1)}+\int_{\Lambda_2}^{\infty} d\gamma\ p(\lambda-\gamma)\rho_N^{(2)}(\gamma)-\frac{1}{2N}p(\lambda-\Lambda_2)\\ &- \frac{p^{'}(\lambda-\Lambda_2)}{12N^2\rho_N^{(2)}(\Lambda_2)}\end{aligned} \tag{6.37}$$

As before, $\mu\Lambda_1$ and $\mu\Lambda_2$ are the largest sea roots from the two "seas" respectively. From this point, the calculation very closely resembles the details found in Section 2 in [57]. Hence, we omit the details and give only the crucial steps. Note that (6.37) can be written in the standard form of the Wiener-Hopf equation [87] after redefining the terms,

$$\begin{aligned}\chi^{(1)}(t)+\chi^{(2)}(t) &- \int_0^{\infty} ds\ p(t-s)\chi^{(1)}(s)-\int_0^{\infty} ds\ p(t-s)\chi^{(2)}(s)\\ &\approx f^{(1)}(t)-\frac{1}{2N}p(t)+\frac{1}{12N^2\rho_N^{(1)}(\Lambda_1)}p^{'}(t)\\ &+ f^{(2)}(t)-\frac{1}{2N}p(t)+\frac{1}{12N^2\rho_N^{(2)}(\Lambda_2)}p^{'}(t)\end{aligned} \tag{6.38}$$

where the following definitions have been adopted

$$\begin{aligned}\chi^{(l)}(\lambda) &= \rho_N^{(l)}(\lambda+\Lambda_l)\\ f^{(l)}(\lambda) &= \rho_\infty^{(l)}(\lambda+\Lambda_l)\end{aligned} \tag{6.39}$$

and following change in variable is used : $t=\lambda-\Lambda_l$ with $l=1,2$ From the Fourier transformed version of (6.38), one can solve for $X_+^{(l)}(\omega)$ which is the Fourier transfrom of $\chi_+^{(l)}(t)$ that is analytic in the upper half complex plane [29],

$$\begin{aligned}\hat{X}_+^{(l)}(\omega) &= \frac{1}{2N}+\frac{i\omega}{12N^2\rho_N^{(l)}(\Lambda_l)}\\ &+ G_+(\omega)\Big(\frac{ig_1}{12N^2\rho_N^{(l)}(\Lambda_l)}-\frac{1}{2N}-\frac{i\omega}{12N^2\rho_N^{(l)}(\Lambda_l)}+\frac{2G_+(i\pi)e^{-\pi\Lambda_l}}{\pi-i\omega}\Big)\end{aligned} \tag{6.40}$$

[29] Again for complete details, refer to [57]

where $G_+(\omega)G_+(-\omega) = 1 + \hat{a}_2(\omega)$ and $g_1 = \frac{i}{12}(2 + \nu - \frac{2\nu}{\nu-1})$. For later use, note that $G_+(0)^2 = \frac{2(\nu-1)}{\nu}$.

From (6.12), (6.39) and (6.40), one can then determine $\rho_N^{(1)}(\Lambda_l)$ and $\rho_N^{(2)}(\Lambda_2)$ explicitly from

$$\chi_+^{(l)}(0) \equiv \frac{1}{2}\rho_N^{(l)}(\Lambda_l) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\ \hat{X}_+^{(l)}(\omega) \tag{6.41}$$

by contour integration and some algebra. We give the result below

$$\rho_N^{(l)}(\Lambda_l) = \frac{1}{4N}\Big\{\pi + 2\pi\alpha + ig_1 + [\pi^2 + \frac{2ig_1\pi}{3} - \frac{g_1^2}{3} + 4\pi^2\alpha^2 + 4\pi\alpha(\pi + ig_1)]^{\frac{1}{2}}\Big\} \tag{6.42}$$

where $\alpha = \frac{1}{G_+(0)} = (\frac{\nu}{2(\nu-1)})^{\frac{1}{2}}$

Finally, using $\rho_\infty^{(l)}(\lambda) \approx 2e^{-\pi\lambda}$ for $\lambda \to \Lambda_l$ and (6.36), one arrives at the desired expression for $1/N$ correction to the energy,

$$E_N - E_\infty = E_{Casimir} = -\frac{\pi^2 \sin\mu}{24\mu N}(1 - 12\alpha^2) \tag{6.43}$$

where the effective central charge is

$$\begin{aligned} c_{eff} &= 1 - 12\alpha^2 \\ &= 1 - 6\frac{\nu}{(\nu-1)} \end{aligned} \tag{6.44}$$

We see that for this model, the central charge, $c = 1$ (Free boson). Also c_{eff} is independent of boundary parameters, unlike for the Dirichlet case [57]. This is a feature expected for models with Neumann boundary condition. Further, from conformal field theory, one also has the following for the conformal dimensions,

$$\begin{aligned} \Delta &= \frac{1 - c_{eff}}{24} \\ &= \frac{\nu}{4(\nu-1)} \end{aligned} \tag{6.45}$$

Note that the above results are derived for the lowest energy state for even N with one hole for each $Q_a(u)$. Reviewing the derivation above, one can notice that the results above can be further generalized for any N and for low lying excited states with arbitrary number of holes, provided these holes are located to the right of the largest sea root as mentioned in the beginning of Section 6.2. For these excited states, the sum for $S_N^{(l)}(\lambda)$ in (6.32) - (6.35) will inevitably have different limits since the number of sea roots vary. However, after applying the Euler-Maclaurin formula, one would recover (6.36) and (6.37). In addition to that, for states with N_H number of holes (all located to the right of the largest sea root), one uses the more general result for the sum rule, namely (6.14) and (6.21) which eventually yields

$$\alpha = \frac{N_H}{G_+(0)} \tag{6.46}$$

Thus, we have the following for the effective central charge and conformal dimensions for low lying excited states

$$\begin{aligned} c_{eff} &= 1 - 6\frac{\nu}{(\nu-1)}N_H^2 \\ \Delta &= \frac{\nu}{4(\nu-1)}N_H^2 \end{aligned} \tag{6.47}$$

Surprisingly, the results (6.45) and (6.47) appear to have more resemblance to spin chains with diagonal boundary terms, as one could see from the $\frac{\nu}{\nu-1}$ dependance [78]-[81], rather than $\frac{\nu-1}{\nu}$ [43] which is the anticipated form for conformal dimensions for spin chains with nondiagonal boundary terms. Indeed the theory of a free Bosonic field φ compactified on a circle of radius r is invariant under $\varphi \mapsto \varphi + 2\pi r$, where $r = \frac{2}{\beta}$. β is the continuum bulk coupling constant that is related to ν by $\beta^2 = 8\pi(\frac{\nu-1}{\nu})$. Further, the quantization of the momentum zero-mode Π_0, yields $\Pi_0 = \frac{n\beta}{2}$ for Neumann boundary condition and $\Pi_0 = \frac{2n}{\beta}$ for the Dirichlet case, where n is an integer. Hence, the zero-mode contribution to the energy, $E_{0,n} \sim \Pi_0^2$ implies $E_{0,n} \sim \Delta \sim (\frac{\nu-1}{\nu})$ for Neumann and $E_{0,n} \sim \Delta \sim (\frac{\nu}{\nu-1})$ for Dirichlet case respectively. More complete discussion on this topic can be found in [43, 80]. Next, we will resort to numerical analysis to confirm our analytical results obtained in this section.

6.3 Numerical results

We present here some numerical results for both odd and even N cases, to support our analytical derivations in Section 6.2.2. We first solve numerically the Bethe equations (6.1), (4.55), (4.56), (6.7) and (6.8) for some large number of spins. We use these solutions to calculate Casimir energy numerically from the following

$$E = E_{bulk} + E_{boundary} + E_{Casimir} \tag{6.48}$$

In (6.48), E is given by (6.11). Thus, having determined the Bethe roots numerically, one uses known expressions for E_{bulk} [13] and $E_{boundary}$ [53] to determine $E_{Casimir}$. Then using the expression found above for $E_{Casimir}$, namely (6.43), one can determine the effective central charge, c_{eff} for that value of N,

$$c_{eff} = -\frac{24\mu N}{\pi^2 \sin\mu}(E - E_{bulk} - E_{boundary}) \tag{6.49}$$

Finally, we employ an algorithm due to Vanden Broeck and Schwartz [83, 84] to extrapolate these values for central charge at $N \to \infty$ limit. Table 6.1 below shows the c_{eff} values for some finite even N, for the lowest energy state with one hole ($N_H = 1$). Equation (6.47) predicts c_{eff} values of -11 and -7 for $p = 1$ and $p = 3$ [30] respectively which are the extrapolated values (-11.000315 and -7.000410) we obtain from the Vanden Broeck and Schwartz method.

For odd N sector, since $N_H = 0$, (6.47) predicts $c_{eff} = 1$ (for the ground state) for any odd p. We present similar numerical results for odd N in Table 6.2 below for $p = 1$ and $p = 3$. We work out the c_{eff} values numerically for $N =$ 15 ,25 ,... ,65. Excellent agreement between the calculated and the extrapolated values of 1.000770 and 1.001851 again strongly supports our analytical results.

[30] $\nu = p + 1$

N	c_{eff}, $p=1\,,\nu=2$	c_{eff}, $p=3\,,\nu=4$
16	-9.365620	-2.853872
24	-9.857713	-3.271279
32	-10.122128	-3.557148
40	-10.287160	-3.770882
48	-10.399970	-3.939554
56	-10.481956	-4.077652
64	-10.544233	-4.193784
$\vdots$	$\vdots$	$\vdots$
∞	-11.000315	-7.000410

Table 6.1: Central charge values, c_{eff} for $p = 1$ ($a_+ = 0.783$, $a_- = 0.859$) and $p = 3$ ($a_+ = 2.29$, $a_- = 1.76$), from numerical computations based on $N = 16\,,24\,,\ldots\,,64$ and extrapolated values at $N \to \infty$ limit (Vanden Broeck and Schwartz algorithm).

N	c_{eff}, $p=1\,,\nu=2$	c_{eff}, $p=3\,,\nu=4$
15	0.898334	0.531501
25	0.936128	0.634012
35	0.953433	0.692758
45	0.963360	0.731841
55	0.969797	0.760142
65	0.974311	0.781795
$\vdots$	$\vdots$	$\vdots$
∞	1.000770	1.001851

Table 6.2: Central charge values, c_{eff} for $p = 1$ ($a_+ = 0.926$, $a_- = 0.654$) and $p = 3$ ($a_+ = 2.10$, $a_- = 1.80$), from numerical computations based on $N = 15\,,25\,,\ldots\,,65$ and extrapolated values at $N \to \infty$ limit (Vanden Broeck and Schwartz algorithm).

From the proposed Bethe equations for an open XXZ spin chain with nondiagonal boundary terms, we computed finite size effect, namely the $1/N$ correction (Casimir energy) to the lowest energy state for both even and odd N. We also studied the bulk excitations due to holes. We found some peculiar results for these excitations of this model. Firstly, the number of holes for excited states seem to be reversed: even number of holes for chains with odd number of spins and vice versa. However, one could explain this by resorting to heuristic arguments involving effects of magnetic fields on the spins at the boundary. We then computed the energy due to hole-excitations. We further generalized the finite-size correction calculation to include multi-hole excited states, where these holes are situated to the right of the largest sea root. Having found the correction, we proceeded to compute the effective central charge, c_{eff} and the conformal dimensions, Δ for the model. We found the central charge, $c = 1$. The effective central charge is independent of the boundary parameters, as expected for models with Neumann boundary condition. The result for Δ however, turns out to be similar to models with diagonal boundary terms rather than the nondiagonal ones, to which the model studied here belongs to.

As an independent check to our analytical results, we also solved the model numerically for some large values of N. We used this solution to compute $1/N$ correction for these large N values, then extrapolate them to the $N \to \infty$ limit using Vanden Broeck and Schwartz algorithm. Our numerical results strongly support the analytical derivations presented here. Hence, the question about the "Dirichlet-like" behaviour remains for now.

There are many other open questions that one can explore and address further. For example, similar analysis involving boundary excitations can also be carried out. This can be really challenging even for the diagonal (Dirichlet) case [79, 89]. Further, solution for more general XXZ model involving multiple $Q(u)$ functions [60, 61], can also be utilized in similar capacity to explore these effects. Last but not least, excitations due to other objects that we choose to ignore here, such as special roots/holes and so forth can also be explored for these models in order to make the study more complete.

Chapter 7: Boundary S Matrix

Factorizable S matrix is an important object of integrable field theories and integrable quantum spin chains. As for the "bulk" case where the S matrix is determined in terms of two-particle scattering amplitudes, the "boundary" case can equally well be formulated in terms of an analogous "one-particle boundary-reflection" amplitude. These bulk and boundary amplitudes are required to satisfy Yang-Baxter [1, 2, 3] and the boundary Yang-Baxter [5, 6] equations respectively. Methods based on Bethe equations have long been used to compute bulk two-particle S matrices [21, 90, 91]. In [21], Fadeev and Takhtajan studied scattering of spinons for the periodic XXX chain for both the ferromagnetic and antiferromagnetic cases. The bulk two-particle S matrix for the latter case coincides with the bulk S matrix for the sine-Gordon model [3] in the limit $\beta^2 \to 8\pi$, where β is the sine-Gordon coupling constant. Much work has also been done on the subject for open spin chains [42, 43, 78, 79], [92]–[95] as well as for integrable field theories with boundary [6, 92]. In [6], Ghoshal and Zamolodchikov presented a precise formulation of the concept of boundary S matrix for $1 + 1$ dimensional quantum field theory with boundaries such as Ising field theory with boundary magnetic field and boundary sine-Gordon model. For the latter model, the authors used a bootstrap approach to compute the boundary S matrix. They determined the scalar factor up to a CDD-type of ambiguity. Nonlinear integral equation (NLIE) [73, 74, 96] approach has also been used to study excitations in integrable quantum field theories such as the sine-Gordon model [75]–[77],[97, 98] and open quantum spin-1/2 XXZ spin chains [42, 43, 78, 79]. In fact, in [43], NLIE approach is used to compute boundary S matrix for the open spin-1/2 XXZ spin chain with nondiagonal boundary terms, where the boundary parameters obey certain constraint. The bulk anisoptopy parameter however is taken to be arbitrary.

In this chapter, we compute the eigenvalues of the boundary S matrix for a special case of an open spin-1/2 XXZ spin chain with nondiagonal boundary terms with two independant boundary parameters (with no constraint) at roots of unity, using the solution obtained recently [51, 53]. The motivation for the performed computation is the fact that the Bethe Ansatz equation for this model is unchanged under sign reversal of the boundary parameters. Hence, the usual trick of obtaining the second eigenvalue of the boundary S matrix of an open spin-1/2 XXZ spin chain by exploiting the change in Bethe Ansatz equation under such sign reversal of the boundary parameters [43, 93, 94, 95] would not work here. Consequently, identifications of separate one-hole states are necessary here. We follow the approach used earlier for diagonal open spin chains [93, 94]. This is a generalization of the method developed by Korepin, Andrei and Destri [90, 91] for computing bulk S matrix. The quantization condition discussed by Fendley and Saleur [92] is a crucial step for the calculation. The solution utilized here was derived for certain values of bulk anisotropy parameter, μ in the repulsive regime ($\mu = \frac{\pi}{p+1} \in (0, \frac{\pi}{2}]$) for odd p values. Hence, we focus only on the critical and repulsive regime, which corresponds in the sine-Gordon model to $\beta^2 \in [4\pi, 8\pi)$ [31]. One-hole excitations for this model occur in even N sector [99] in contrast to the diagonal open spin-1/2 XXZ spin chain where such excitations appear in the odd N sector [94].

Since the Bethe roots for the model consist of “sea” roots and “extra” roots, we rely on a conjectured relation between the “extra” roots and the hole rapidity,

[31] $\beta^2 = 8(\pi - \mu)$

which is confirmed numerically for system up to about 60 sites. We find that the eigenvalue derived for the open XXZ spin chain agrees with one of the eigenvalues of Ghoshal-Zamolodchikov's boundary S matrix for the one boundary sine-Gordon model, provided the lattice boundary parameters that appear in the spin chain Hamiltonian and the IR parameters that appear in Ghoshal-Zamolodchikov's boundary S matrix [6] obey the same relation as in [43] [32]. The problem of finding the second eigenvalue of the boundary S matrix requires the identification of an independent one-hole state. In contrast to previous studies [43, 93, 94, 95], where such state was found by reversing the signs of the boundary parameters [33], similar strategy does not work here. Reversing the signs of the boundary parameters in the present case leaves the Bethe equation unchanged, hence giving the same one-hole state. Interestingly, a separate one-hole state with 2-string is found [99]. Using a conjectured relation between "extra" roots, hole rapidity and the boundary parameters, which is again confirmed numerically for system up to about 60 sites, we derive the remaining eigenvalue which also agrees with Ghoshal-Zamolodchikov's result.

7.1 One-hole state

In order to compute the spinon boundary scattering amplitude, we consider a one-hole state. The roots distribution for such a state was found in [53]. One-hole excitations for the open XXZ spin chain we study here appear in the even N sector. Hence, it is sufficient to consider the results for even N case. The shifted Bethe roots $\tilde{u}_j^{(a)} = u_j^{(a)} + \frac{\eta}{2}$ for this state have the form (4.51). The Bethe Ansatz

[32] Very recently, similar relations were found for the open XXZ spin chain with diagonal-nondiagonal boundary terms in [95].

[33] In fact, there is a change $\xi_\pm \to -\xi_\pm$ in the Bethe equation for the diagonal case [94].

equations are re-expressed in terms of counting functions, $\mathsf{h}^{(l)}(\lambda)$ as

$$\mathsf{h}^{(l)}(\lambda_j^{(l,1)}) = J_j, \quad l = 1\,,2 \tag{7.1}$$

where $\mathsf{h}^{(l)}(\lambda)$ are given by (4.55) and (4.56). Further, $\{J_1, J_2, \ldots, J_{\frac{N}{2}}\}$ is a set of increasing positive integers that parametrize the state [34]. For states with no holes, the integers take consecutive values. For one-hole state, there is a break in the sequence, represented by a missing integer. This missing integer $\tilde{J}$, fixes the value of the hole rapidity, $\tilde{\lambda}$, according to

$$\mathsf{h}^{(1)}(\tilde{\lambda}) = \mathsf{h}^{(2)}(\tilde{\lambda}) = \tilde{J}. \tag{7.2}$$

If the hole is located to the right of the largest "sea" root $(\lambda_{\frac{N}{2}}^{(a,1)})$, then $\tilde{J} = \lfloor \mathsf{h}^{(l)}(\infty) - \mathsf{h}^{(l)}(\lambda_{\frac{N}{2}}^{(a,1)}) \rfloor$. See [99] for more details. For later use, we next define the densities of sea roots as

$$\rho^{(l)}(\lambda) = \frac{1}{N}\frac{d\mathsf{h}^{(l)}(\lambda)}{d\lambda} \tag{7.3}$$

where $l = 1\,,2$

7.2 One-hole state with 2-string

In addition to the one-hole state mentioned in last section, there is another one-hole state. This state is the only remaining one-hole state, which also has a 2-string. In this section, we give some brief information on the state. The shifted Bethe roots $\tilde{u}_j^{(a)} = u_j^{(a)} + \frac{\eta}{2}$ for this state have the following form

$$\begin{cases} \mu\lambda_j^{(a,1)} & j = 1\,,2\,,\ldots\,,M_{(a,1)} \\ \mu\lambda_j^{(a,2)} + \frac{i\pi}{2}\,, & j = 1\,,2\,,\ldots\,,M_{(a,2)} \\ \mu\lambda_0^{(a)} + \frac{\eta}{2} & \\ \mu\lambda_0^{(a)} - \frac{\eta}{2} & \end{cases}\,, \qquad a = 1\,,2\,, \tag{7.4}$$

[34] In principle, there are two such sets of integers, $\left\{J_i^{(1)}\right\}$ and $\left\{J_i^{(2)}\right\}$ corresponding to the two counting functions, $\mathsf{h}^{(1)}(\lambda)$ and $\mathsf{h}^{(2)}(\lambda)$ respectively. But, in fact these two sets of integers are identical. Hence we choose to drop the superscript, l from J_j in (7.1).

where $\lambda_0^{(a)}$, $\mu = \frac{\pi}{p+1}$ and $\lambda_j^{(a,b)}$ are real. Here, $M_{(1,1)} = M_{(2,1)} = \frac{N}{2} - 1$, and $M_{(1,2)} = \frac{p-1}{2}$, $M_{(2,2)} = \frac{p-3}{2}$. As before, $\mu\lambda_j^{(a,1)}$ are the zeros of $Q_a(u)$ that form real sea ("sea" roots) and $\mu\lambda_k^{(a,2)}$ are real parts of the "extra" roots (also zeros of $Q_a(u)$) which are not part of the "seas." For this state, we also have $\mu\lambda_0^{(a)}$, the real parts of additional "extra" roots that form a 2-string.

The counting functions for this state are given by

$$\begin{aligned}\mathsf{h}^{(1)}(\lambda) = \frac{1}{2\pi}\Big\{&(2N+1)q_1(\lambda) - r_1(\lambda) - q_{1+2a_-}(\lambda) - q_{1-2a_-}(\lambda) - q_{1+2a_+}(\lambda) - q_{1-2a_+}(\lambda)\\ &- \sum_{k=1}^{\frac{N}{2}-1}\Big[q_2(\lambda - \lambda_k^{(2,1)}) + q_2(\lambda + \lambda_k^{(2,1)})\Big] - \sum_{k=1}^{(p-3)/2}\Big[r_2(\lambda - \lambda_k^{(2,2)}) + r_2(\lambda + \lambda_k^{(2,2)})\Big]\\ &-q_3(\lambda - \lambda_0^{(2)}) - q_3(\lambda + \lambda_0^{(2)}) - q_1(\lambda - \lambda_0^{(2)}) - q_1(\lambda + \lambda_0^{(2)})\Big\}\,,\end{aligned} \tag{7.5}$$

and

$$\begin{aligned}\mathsf{h}^{(2)}(\lambda) = \frac{1}{2\pi}\Big\{&(2N+1)q_1(\lambda) - r_1(\lambda)\\ &- \sum_{k=1}^{\frac{N}{2}-1}\Big[q_2(\lambda - \lambda_k^{(1,1)}) + q_2(\lambda + \lambda_k^{(1,1)})\Big] - \sum_{k=1}^{(p-1)/2}\Big[r_2(\lambda - \lambda_k^{(1,2)}) + r_2(\lambda + \lambda_k^{(1,2)})\Big]\\ &-q_3(\lambda - \lambda_0^{(1)}) - q_3(\lambda + \lambda_0^{(1)}) - q_1(\lambda - \lambda_0^{(1)}) - q_1(\lambda + \lambda_0^{(1)})\Big\}\,.\end{aligned} \tag{7.6}$$

The Bethe Ansatz equations for this state take the following form,

$$\mathsf{h}^{(l)}(\lambda_j^{(l,1)}) = J_j, \quad l = 1\,,2 \tag{7.7}$$

where $\{J_1, J_2, \ldots, J_{\frac{N}{2}-1}\}$ is a set of increasing positive integers that parametrize the state. The hole for this state breaks the sequence, represented by a missing integer. As before, the missing integer $\tilde{J}$,enables one to calculate the hole rapidity, $\tilde{\lambda}$ using

$$\mathsf{h}^{(1)}(\tilde{\lambda}) = \mathsf{h}^{(2)}(\tilde{\lambda}) = \tilde{J}. \tag{7.8}$$

If the hole appears to the right of the largest "sea" root ($\lambda_{\frac{N}{2}-1}^{(a,1)}$), then $\tilde{J} = \lfloor \mathsf{h}^{(l)}(\infty) - \mathsf{h}^{(l)}(\lambda_{\frac{N}{2}-1}^{(a,1)}) \rfloor$. More on this state can be found in [99].

7.3 Boundary S matrix

In this Section, we give the derivation for the boundary scattering amplitudes for one-hole states reviewed in Section 6.1.

7.3.1 Eigenvalue for the one-hole state without 2-string

First, we consider the state reviewed in Section 7.1. From (4.55), (4.56), (7.3) and (4.26), one can solve for the sum of the two densities. We recall the results below [53],

$$\begin{aligned} \rho_{total}(\lambda) &= \rho^{(1)}(\lambda) + \rho^{(2)}(\lambda) \\ &= 4s(\lambda) + \frac{1}{N} R_+(\lambda) \end{aligned} \tag{7.9}$$

where $s(\lambda) = \frac{1}{2\cosh(\pi\lambda)}$ and $R_+(\lambda)$ is the inverse Fourier transform of $\hat{R}_+(\omega)$ which is given by

$$\begin{aligned} \hat{R}_+(\omega) &= \frac{1}{1+\hat{a}_2(\omega)} \Big[2\hat{a}_1(\omega) + 2\hat{a}_2(\omega) - 2\hat{b}_1(\omega) - \hat{a}_{1+2a_-}(\omega) - \hat{a}_{1-2a_-}(\omega) \\ &- \hat{a}_{1+2a_+}(\omega) - \hat{a}_{1-2a_+}(\omega) - 2\hat{b}_2(\omega)\Big(\sum_{k=1}^{\frac{p-1}{2}} \cos(\lambda_k^{(2,2)}\omega) + \sum_{l=1}^{\frac{p+1}{2}} \cos(\lambda_l^{(1,2)}\omega)\Big) \\ &+ 4\hat{a}_2(\omega)\cos(\tilde{\lambda}\omega) \Big] \end{aligned} \tag{7.10}$$

The presence of extra roots, $\lambda_k^{(a,2)}$ and the hole rapidity, $\tilde{\lambda}$, are to be noted here[35]. Henceforth, we shall denote $\lambda_k^{(a,2)}$ simply as $\lambda_k^{(a)}$. Morever, momentum of the excitation is given by

$$p(\tilde{\lambda}) = \tan^{-1}\left(\sinh(\pi\tilde{\lambda})\right) - \frac{\pi}{2} \tag{7.11}$$

From (7.11), one gets $s(\lambda) = \frac{1}{2\pi}\frac{dp(\lambda)}{d\lambda}$. Consequently, using (7.3), one rewrites (7.9) as

$$\frac{1}{N}\frac{d\mathsf{h}_{total}(\lambda)}{d\lambda} = \frac{2}{\pi}\frac{dp(\lambda)}{d\lambda} + \frac{1}{N}R_+(\lambda) \tag{7.12}$$

[35] Energy carried by the hole is given by $E(\tilde{\lambda}) = \frac{\pi \sin\mu}{2\mu}\frac{1}{\cosh(\pi\tilde{\lambda})}$. Such an expression for spinon was derived in [21]

where $\mathsf{h}_{total}(\lambda) = \mathsf{h}^{(1)}(\lambda) + \mathsf{h}^{(2)}(\lambda)$ and $\frac{1}{N}\frac{d\mathsf{h}_{total}(\lambda)}{d\lambda} = \rho_{total}(\lambda)$. After integrating (7.12) with respect to λ, taking limits of integration from 0 to $\tilde{\lambda}$, one finds [36]

$$\mathsf{h}_{total}(\tilde{\lambda}) = \mathsf{h}^{(1)}(\tilde{\lambda}) + \mathsf{h}^{(2)}(\tilde{\lambda}) = \frac{2}{\pi}Np(\tilde{\lambda}) + \int_0^{\tilde{\lambda}} d\lambda R_+(\lambda) \tag{7.13}$$

Since $\mathsf{h}^{(1)}(\tilde{\lambda}) = \mathsf{h}^{(2)}(\tilde{\lambda}) \in$ positive integer and $R_+(\lambda)$ is an even function of λ, multiplying the resulting expression by $2i\pi$ and exponentiating gives

$$e^{2ip(\tilde{\lambda})N} e^{\frac{i\pi}{2}\int_{-\tilde{\lambda}}^{\tilde{\lambda}} d\lambda R_+(\lambda)} = 1 \tag{7.14}$$

Next, let us compare equation (7.14) to the Yang's quantization condition for a particle on an interval of length N,

$$e^{2ip(\tilde{\lambda})N} R(\tilde{\lambda}; a_+) R(\tilde{\lambda}; a_-) \mid \tilde{\lambda}, (\pm)\rangle = \mid \tilde{\lambda}, (\pm)\rangle \tag{7.15}$$

where $R(\tilde{\lambda}; a_\pm)$ are the non-diagonal boundary S matrices and $\mid \tilde{\lambda}, (\pm)\rangle$ denote the two possible one-hole states. Note that the $\pm$ in $\mid \tilde{\lambda}, (\pm)\rangle$ represents two posssible one-hole states and not the right and left boundaries. The expression $e^{\frac{i\pi}{2}\int_{-\tilde{\lambda}}^{\tilde{\lambda}} d\lambda R_+(\lambda)}$ then, should be equal to one of the two eigenvalues of the Yang matrix $Y(\tilde{\lambda})$ defined by

$$Y(\tilde{\lambda}) = R(\tilde{\lambda}; a_+) R(\tilde{\lambda}; a_-) \tag{7.16}$$

Defining this eigenvalue as $\alpha(\tilde{\lambda}, a_+)\alpha(\tilde{\lambda}, a_-)$, where $+$ and $-$ denote the right and left boundaries respectively, (7.14) can be rephrased as

$$e^{2ip(\tilde{\lambda})N} \alpha(\tilde{\lambda}, a_+)\alpha(\tilde{\lambda}, a_-) = 1 \tag{7.17}$$

The problem thus reduces to evaluating the following

$$\alpha(\tilde{\lambda}, a_+)\alpha(\tilde{\lambda}, a_-) = e^{\frac{i\pi}{2}\int_{-\tilde{\lambda}}^{\tilde{\lambda}} d\lambda R_+(\lambda)} \tag{7.18}$$

[36]Since we are only able to determine the scattering amplitudes up to a rapidity-independent factor, the additive constant $p(0)$ from the integration is ignored in (7.13).

After some manipulations, we have the following,

$$\begin{aligned}\alpha(\tilde{\lambda}, a_+)\alpha(\tilde{\lambda}, a_-) &= \exp\Big\{2\int_0^\infty \frac{d\omega}{\omega}\sinh(2i\tilde{\lambda}\omega)\Big[\frac{\hat{a}_2(\omega)}{1+\hat{a}_2(\omega)} + \frac{1}{1+\hat{a}_2(2\omega)}[\hat{a}_2(2\omega) \\ &+ \hat{a}_1(2\omega) - \hat{b}_1(2\omega) - \frac{1}{2}(\hat{a}_{1+2a_-}(2\omega) + \hat{a}_{1-2a_-}(2\omega) \\ &+ \hat{a}_{1+2a_+}(2\omega) + \hat{a}_{1-2a_+}(2\omega)) \\ &- \hat{b}_2(2\omega)(\sum_{k=1}^{\frac{p-1}{2}}\cos(2\lambda_k^{(2)}\omega) + \sum_{l=1}^{\frac{p+1}{2}}\cos(2\lambda_l^{(1)}\omega))]\Big]\Big\}\end{aligned} \quad (7.19)$$

Further, using (4.30) and (4.31), one gets

$$\begin{aligned}\alpha(\tilde{\lambda}, a_+)\alpha(\tilde{\lambda}, a_-) &= \exp\Big\{2\int_0^\infty \frac{d\omega}{\omega}\sinh(2i\tilde{\lambda}\omega)\Big[\frac{2\sinh(3\omega/2)\sinh((\nu-2)\omega/2)}{\sinh(2\omega)\sinh((\nu-1)\omega/2)} \\ &+ \frac{\sinh(\omega)}{\sinh((\nu-1)\omega)\cosh(\omega)} + \frac{\sinh((-\nu+2a_- -1)\omega)}{2\sinh((\nu-1)\omega)\cosh(\omega)} \\ &+ \frac{\sinh((\nu-2a_- -1)\omega)}{2\sinh((\nu-1)\omega)\cosh(\omega)} + (a_- \to a_+) \\ &+ \frac{\sinh(\omega)}{\sinh((\nu-1)\omega)}(\sum_{k=1}^{\frac{p-1}{2}}\cos(2\lambda_k^{(2)}\omega) + \sum_{l=1}^{\frac{p+1}{2}}\cos(2\lambda_l^{(1)}\omega))\Big]\Big\}\end{aligned} \quad (7.20)$$

where $(a_- \to a_+)$ is a shorthand for two additional terms which are the same as the third and fourth terms in the integrand of (7.20), but with a_- replaced by a_+. The integrals involving "extra" roots $\lambda_k^{(2)}$ and $\lambda_l^{(1)}$ yield

$$\begin{aligned}&\exp\Big\{2\int_0^\infty \frac{d\omega}{\omega}\sinh(2i\tilde{\lambda}\omega)\frac{\sinh(\omega)}{\sinh((\nu-1)\omega)}(\sum_{k=1}^{\frac{p-1}{2}}\cos(2\lambda_k^{(2)}\omega) + \sum_{l=1}^{\frac{p+1}{2}}\cos(2\lambda_l^{(1)}\omega))\Big\} \\ &\qquad = \prod_{k=1}^{\frac{p-1}{2}}\prod_{l=1}^{\frac{p+1}{2}}\sqrt{f(\lambda_k^{(2)}, \lambda_l^{(1)}, \tilde{\lambda})f(\lambda_k^{(2)}, \lambda_l^{(1)}, \tilde{\lambda}+\frac{i\pi}{\mu'})}\end{aligned} \quad (7.21)$$

where $\mu' = \frac{\pi}{\nu-1}$ and

$$\begin{aligned}f(\lambda_k^{(2)}, \lambda_l^{(1)}, \tilde{\lambda}) &= \frac{\sinh\left(\frac{\mu'}{2}(\tilde{\lambda}+\lambda_k^{(2)}+\frac{i}{2}-\frac{i\pi}{2\mu'})\right)\cosh\left(\frac{\mu'}{2}(\tilde{\lambda}-\lambda_k^{(2)}+\frac{i}{2}+\frac{i\pi}{2\mu'})\right)}{\sinh\left(\frac{\mu'}{2}(\tilde{\lambda}+\lambda_k^{(2)}-\frac{i}{2}+\frac{i\pi}{2\mu'})\right)\cosh\left(\frac{\mu'}{2}(\tilde{\lambda}-\lambda_k^{(2)}-\frac{i}{2}-\frac{i\pi}{2\mu'})\right)} \\ &\times \frac{\sinh\left(\frac{\mu'}{2}(\tilde{\lambda}+\lambda_l^{(1)}+\frac{i}{2}+\frac{i\pi}{2\mu'})\right)\cosh\left(\frac{\mu'}{2}(\tilde{\lambda}-\lambda_l^{(1)}+\frac{i}{2}-\frac{i\pi}{2\mu'})\right)}{\sinh\left(\frac{\mu'}{2}(\tilde{\lambda}+\lambda_l^{(1)}-\frac{i}{2}-\frac{i\pi}{2\mu'})\right)\cosh\left(\frac{\mu'}{2}(\tilde{\lambda}-\lambda_l^{(1)}-\frac{i}{2}+\frac{i\pi}{2\mu'})\right)}\end{aligned} \quad (7.22)$$

After evaluating the rest of the integrals, (7.20) becomes

$$\begin{aligned}\alpha(\tilde{\lambda}, a_+)\alpha(\tilde{\lambda}, a_-) &= S_0(\tilde{\lambda})^2 S_1(\tilde{\lambda}, a_-) S_1(\tilde{\lambda}, a_+) \\ &\times \prod_{k=1}^{\frac{p-1}{2}} \prod_{l=1}^{\frac{p+1}{2}} \sqrt{f(\lambda_k^{(2)}, \lambda_l^{(1)}, \tilde{\lambda}) f(\lambda_k^{(2)}, \lambda_l^{(1)}, \tilde{\lambda} + \frac{i\pi}{\mu'})}\end{aligned} \tag{7.23}$$

where

$$\begin{aligned}S_0(\tilde{\lambda}) &= \frac{1}{\pi}\cosh(\mu'\tilde{\lambda}) \prod_{n=0}^{\infty} \frac{\Gamma\left[\frac{1}{\nu-1}(4n+1-2i\tilde{\lambda})\right]\Gamma\left[\frac{1}{\nu-1}(4n+3-2i\tilde{\lambda})+1\right]}{\Gamma\left[\frac{1}{\nu-1}(4n+1+2i\tilde{\lambda})\right]\Gamma\left[\frac{1}{\nu-1}(4n+3+2i\tilde{\lambda})+1\right]} \\ &\times \frac{\Gamma\left[\frac{1}{\nu-1}(4n+4+2i\tilde{\lambda})\right]\Gamma\left[\frac{1}{\nu-1}(4n+2i\tilde{\lambda})+1\right]}{\Gamma\left[\frac{1}{\nu-1}(4n+4-2i\tilde{\lambda})\right]\Gamma\left[\frac{1}{\nu-1}(4n-2i\tilde{\lambda})+1\right]} \\ &\times \frac{\Gamma^2\left[\frac{1}{\nu-1}(2n-i\tilde{\lambda})+\frac{1}{2}\right]\Gamma^2\left[\frac{1}{\nu-1}(2n+1+i\tilde{\lambda})+\frac{1}{2}\right]}{\Gamma^2\left[\frac{1}{\nu-1}(2n+2+i\tilde{\lambda})+\frac{1}{2}\right]\Gamma^2\left[\frac{1}{\nu-1}(2n+1-i\tilde{\lambda})+\frac{1}{2}\right]}\end{aligned} \tag{7.24}$$

$$\begin{aligned}S_1(\tilde{\lambda}, a_\pm) &= \frac{1}{\pi}\sqrt{\cosh(\mu'(\tilde{\lambda} + \frac{i}{2}(\nu - 2a_\pm)))\cosh(\mu'(\tilde{\lambda} - \frac{i}{2}(\nu - 2a_\pm)))} \\ &\times \prod_{n=0}^{\infty} \frac{\Gamma\left[\frac{1}{\nu-1}(2n+1+i\tilde{\lambda}-\frac{1}{2}(\nu-2a_\pm))+\frac{1}{2}\right]}{\Gamma\left[\frac{1}{\nu-1}(2n+1-i\tilde{\lambda}-\frac{1}{2}(\nu-2a_\pm))+\frac{1}{2}\right]} \\ &\times \frac{\Gamma\left[\frac{1}{\nu-1}(2n+1+i\tilde{\lambda}+\frac{1}{2}(\nu-2a_\pm))+\frac{1}{2}\right]}{\Gamma\left[\frac{1}{\nu-1}(2n+1-i\tilde{\lambda}+\frac{1}{2}(\nu-2a_\pm))+\frac{1}{2}\right]} \\ &\times \frac{\Gamma\left[\frac{1}{\nu-1}(2n-i\tilde{\lambda}-\frac{1}{2}(\nu-2a_\pm))+\frac{1}{2}\right]}{\Gamma\left[\frac{1}{\nu-1}(2n+2+i\tilde{\lambda}-\frac{1}{2}(\nu-2a_\pm))+\frac{1}{2}\right]} \\ &\times \frac{\Gamma\left[\frac{1}{\nu-1}(2n-i\tilde{\lambda}+\frac{1}{2}(\nu-2a_\pm))+\frac{1}{2}\right]}{\Gamma\left[\frac{1}{\nu-1}(2n+2+i\tilde{\lambda}+\frac{1}{2}(\nu-2a_\pm))+\frac{1}{2}\right]}\end{aligned} \tag{7.25}$$

The values of the "extra" roots are dependant on the hole rapidity, $\tilde{\lambda}$ and the boundary parameters, $a_\pm$. Hence, it is sensible to expect a relation between these "extra" roots, $\left\{\lambda_k^{(2)}, \lambda_l^{(1)}\right\}$, the boundary parameters, $a_\pm$ and the hole rapidity, $\tilde{\lambda}$. Consequently, one needs to express the right hand side of (7.21) in terms of purely $a_\pm$ and $\tilde{\lambda}$ to complete the derivation. To look for this additional relation, we begin with the information contained in the difference of the two densities, $\rho^{(1)}(\lambda) - \rho^{(2)}(\lambda)$. This leads to the following,

$$\begin{aligned}\rho_{diff}(\lambda) &= \rho^{(1)}(\lambda) - \rho^{(2)}(\lambda) \\ &= \frac{1}{N} R_-(\lambda) \end{aligned} \tag{7.26}$$

where $R_-(\lambda)$ has the following Fourier transform,

$$\begin{aligned}\hat{R}_-(\omega) &= \frac{1}{1-\hat{a}_2(\omega)}\Big[-\hat{a}_{1+2a_-}(\omega) - \hat{a}_{1-2a_-}(\omega) - \hat{a}_{1+2a_+}(\omega) - \hat{a}_{1-2a_+}(\omega) \\ &- 2\hat{b}_2(\omega)\big(\sum_{k=1}^{\frac{p-1}{2}} \cos(\lambda_k^{(2)}\omega) - \sum_{l=1}^{\frac{p+1}{2}} \cos(\lambda_l^{(1)}\omega)\big)\Big] \end{aligned} \tag{7.27}$$

Analogous to (7.12)) one gets

$$\frac{1}{N}\frac{d\mathsf{h}_{diff}(\lambda)}{d\lambda} = \frac{1}{N} R_-(\lambda) \tag{7.28}$$

where $\mathsf{h}_{diff}(\lambda) = \mathsf{h}^{(1)}(\lambda) - \mathsf{h}^{(2)}(\lambda)$ and $\frac{1}{N}\frac{d\mathsf{h}_{diff}(\lambda)}{d\lambda} = \rho_{diff}(\lambda)$. Further, integrating (7.28) with respect to λ, taking limits of integration from 0 to $\tilde{\lambda}$ as before, one finds

$$\mathsf{h}_{diff}(\tilde{\lambda}) = \mathsf{h}^{(1)}(\tilde{\lambda}) - \mathsf{h}^{(2)}(\tilde{\lambda}) = \int_0^{\tilde{\lambda}} d\lambda R_-(\lambda) \tag{7.29}$$

Since $\mathsf{h}^{(1)}(\tilde{\lambda}) = \mathsf{h}^{(2)}(\tilde{\lambda}) \in$ positive integer, using the fact that $R_-(\lambda)$ is an even function of λ and exponentiating (7.29) we get

$$e^{\int_{-\tilde{\lambda}}^{\tilde{\lambda}} d\lambda R_-(\lambda)} = g(\tilde{\lambda}, a_+) g(\tilde{\lambda}, a_-) \prod_{k=1}^{\frac{p-1}{2}} \prod_{l=1}^{\frac{p+1}{2}} \sqrt{\frac{f(\lambda_k^{(2)}, \lambda_l^{(1)}, \tilde{\lambda})}{f(\lambda_k^{(2)}, \lambda_l^{(1)}, \tilde{\lambda} + \frac{i\pi}{\mu'})}} = 1 \tag{7.30}$$

where $g(\tilde{\lambda}, a_\pm) \equiv \sqrt{\frac{\cosh(\frac{i\mu'}{2}(\nu - 2a_\pm)) + i\sinh(\mu'\tilde{\lambda})}{\cosh(\frac{i\mu'}{2}(\nu - 2a_\pm)) - i\sinh(\mu'\tilde{\lambda})}}$. Next, an important observation is the following relation (as $N \to \infty$),

$$\prod_{k=1}^{\frac{p-1}{2}} \prod_{l=1}^{\frac{p+1}{2}} f(\lambda_k^{(2)}, \lambda_l^{(1)}, \tilde{\lambda}) = -1 \tag{7.31}$$

for which we provide numerical support in Table 7.1. Although the results shown in Table 7.1 are computed for the case where the hole appears to the right of the largest "sea" root, we find similar results for other hole locations. From (7.30) and (7.31), it also follows that

$$\prod_{k=1}^{\frac{p-1}{2}} \prod_{l=1}^{\frac{p+1}{2}} f(\lambda_k^{(2)}, \lambda_l^{(1)}, \tilde{\lambda} + \frac{i\pi}{\mu'}) = -\Big(g(\tilde{\lambda}, a_+) g(\tilde{\lambda}, a_-)\Big)^2 \qquad (7.32)$$

N	$\prod_{k=1}^{\frac{p-1}{2}} \prod_{l=1}^{\frac{p+1}{2}} f(\lambda_k^{(2)}, \lambda_l^{(1)}, \tilde{\lambda})$, $p=3$	$\prod_{k=1}^{\frac{p-1}{2}} \prod_{l=1}^{\frac{p+1}{2}} f(\lambda_k^{(2)}, \lambda_l^{(1)}, \tilde{\lambda})$, $p=5$
24	-0.999364 + 0.0356655 i	-0.999334 + 0.036496 i
32	-0.999421 + 0.0340133 i	-0.999333 + 0.036522 i
40	-0.999466 + 0.0326686 i	-0.999334 + 0.036486 i
48	-0.999502 + 0.0315413 i	-0.999337 + 0.036419 i
56	-0.999532 + 0.0305749 i	-0.999340 + 0.036336 i
64	-0.999558 + 0.0297318 i	-0.999343 + 0.036243 i

Table 7.1: $\prod_{k=1}^{\frac{p-1}{2}} \prod_{l=1}^{\frac{p+1}{2}} f(\lambda_k^{(2)}, \lambda_l^{(1)}, \tilde{\lambda})$ for $p = 3$ ($a_+ = 2.1$, $a_- = 1.6$) and $p = 5$ ($a_+ = 3.3$, $a_- = 2.7$), from numerical solutions based on $N = 24, 32, \ldots, 64$.

We stress here that the values of $\lambda_k^{(2)}$ and $\lambda_l^{(1)}$ used in computations above strictly satisfy the Bethe equations (6.1). Finally, we can rewrite (7.23) as

$$\alpha(\tilde{\lambda}, a_+)\alpha(\tilde{\lambda}, a_-) = S_0(\tilde{\lambda})^2 S_1(\tilde{\lambda}, a_-) S_1(\tilde{\lambda}, a_+) g(\tilde{\lambda}, a_+) g(\tilde{\lambda}, a_-) \qquad (7.33)$$

up to a rapidity-independant phase factor. Subsequently, the complete expression for each boundary's scattering amplitude is given by (up to a rapidity-independant phase factor)

$$\alpha(\tilde{\lambda}, a_\pm) = S_0(\tilde{\lambda}) S_1(\tilde{\lambda}, a_\pm) g(\tilde{\lambda}, a_\pm) \qquad (7.34)$$

where $+$ and $-$ again denotes right and left boundaries respectively.

7.3.2 Eigenvalue for the one-hole state with 2-string

We now consider the one-hole state with a 2-string, reviewed in Section 7.2. The computation of the eigenvalue for this state is identical to the one given above.

Hence, we skip the details and present the result. Analogous to (7.20), we have

$$\begin{aligned}
\beta(\tilde{\lambda}, a_+)\beta(\tilde{\lambda}, a_-) &= \exp\Big\{2\int_0^\infty \frac{d\omega}{\omega}\sinh(2i\tilde{\lambda}\omega)\Big[\frac{2\sinh(3\omega/2)\sinh((\nu-2)\omega/2)}{\sinh(2\omega)\sinh((\nu-1)\omega/2)} \\
&+ \frac{\sinh(\omega)}{\sinh((\nu-1)\omega)\cosh(\omega)} + \frac{\sinh((-\nu+2a_--1)\omega)}{2\sinh((\nu-1)\omega)\cosh(\omega)} \\
&+ \frac{\sinh((\nu-2a_--1)\omega)}{2\sinh((\nu-1)\omega)\cosh(\omega)} + (a_- \to a_+) \\
&+ \frac{\sinh(\omega)}{\sinh((\nu-1)\omega)}\Big(\sum_{k=1}^{\frac{p-3}{2}}\cos(2\lambda_k^{(2)}\omega) + \sum_{l=1}^{\frac{p-1}{2}}\cos(2\lambda_l^{(1)}\omega)\Big) \\
&+ \frac{\sinh(2\omega)}{\sinh((\nu-1)\omega)}\big(\cosh(2i\lambda_0^{(1)}\omega) + \cosh(2i\lambda_0^{(2)}\omega)\big)\Big]\Big\} \qquad (7.35)
\end{aligned}$$

which after evaluating the integrals yields

$$\begin{aligned}
\beta(\tilde{\lambda}, a_+)\beta(\tilde{\lambda}, a_-) &= S_0(\tilde{\lambda})^2 S_1(\tilde{\lambda}, a_-) S_1(\tilde{\lambda}, a_+) w(\lambda_0^{(1)}, \tilde{\lambda}) w(\lambda_0^{(2)}, \tilde{\lambda}) \\
&\times \prod_{k=1}^{\frac{p-3}{2}}\prod_{l=1}^{\frac{p-1}{2}}\sqrt{f(\lambda_k^{(2)}, \lambda_l^{(1)}, \tilde{\lambda}) f(\lambda_k^{(2)}, \lambda_l^{(1)}, \tilde{\lambda} + \frac{i\pi}{\mu'})} \qquad (7.36)
\end{aligned}$$

where

$$w(\lambda_0^{(a)}, \tilde{\lambda}) = \sqrt{\frac{\cosh(\mu'(\tilde{\lambda} + \lambda_0^{(a)} + i))}{\cosh(\mu'(\tilde{\lambda} + \lambda_0^{(a)} - i))}\frac{\cosh(\mu'(\tilde{\lambda} - \lambda_0^{(a)} + i))}{\cosh(\mu'(\tilde{\lambda} - \lambda_0^{(a)} - i))}}\,, \quad a = 1\,,2\,, \quad (7.37)$$

As before, $(a_- \to a_+)$ represents two additional terms which are the same as the third and fourth terms in the integrand of (7.35), but with a_- replaced by a_+. We proceed to make the following conjecture to complete the derivation.

$$\begin{aligned}
w(\lambda_0^{(1)}, \tilde{\lambda}) w(\lambda_0^{(2)}, \tilde{\lambda}) \prod_{k=1}^{\frac{p-3}{2}}\prod_{l=1}^{\frac{p-1}{2}}\sqrt{f(\lambda_k^{(2)}, \lambda_l^{(1)}, \tilde{\lambda}) f(\lambda_k^{(2)}, \lambda_l^{(1)}, \tilde{\lambda} + \frac{i\pi}{\mu'})} &= g(\tilde{\lambda} + \frac{i\pi}{\mu'}, a_+) \\
&\times g(\tilde{\lambda} + \frac{i\pi}{\mu'}, a_-)
\end{aligned} \qquad (7.38)$$

Like (7.31), we provide numerical support for (7.38) in Table 7.2 where we compute the ratio $\phi \equiv \frac{d_1}{d_2}$, where d_1 and d_2 are the left hand side and the right hand side of (7.38) respectively, for systems up to 64 sites. We believe this supports the validity of (7.38) at $N \to \infty$. The values of $\lambda_k^{(2)}$, $\lambda_l^{(1)}$, $\lambda_0^{(1)}$ and $\lambda_0^{(2)}$ used in computations are obtained by solving numerically the Bethe equations (7.5) and (7.6) for the "sea" roots and (6.1) for the "extra" roots. The correctness and validity of such numerical solutions are checked by comparing them with the ones obtained from McCoy's method for smaller number of sites, e.g., $N = 2, 4$ and 6 [37]. We stress here that although the results obtained in Table 7.2 are computed for $\tilde{J} = 1$, namely the case where the hole appears close to the origin, similar results are found for other hole locations, e.g., $\tilde{J} = 2, 3, \ldots$.

N	ϕ, $p = 3$	ϕ, $p = 5$
24	0.967073 + 0.254500 i	0.990295 + 0.138982 i
32	0.981063 + 0.193688 i	0.994434 + 0.105361 i
40	0.987716 + 0.156259 i	0.996308 + 0.085849 i
48	0.991392 + 0.130928 i	0.997674 + 0.068166 i
56	0.993634 + 0.112654 i	0.998065 + 0.062174 i
64	0.995102 + 0.098852 i	0.998407 + 0.056428 i

Table 7.2: ϕ for $p = 3$ ($a_+ = 2.1$, $a_- = 1.6$) and $p = 5$ ($a_+ = 3.2$, $a_- = 2.7$), from numerical solutions based on $N = 24, 32, \ldots, 64$.

Using (7.38), the other eigenvalue for the Yang matrix (7.16) becomes

$$\beta(\tilde{\lambda}, a_+)\beta(\tilde{\lambda}, a_-) = S_0(\tilde{\lambda})^2 S_1(\tilde{\lambda}, a_+) S_1(\tilde{\lambda}, a_-) g(\tilde{\lambda} + \frac{i\pi}{\mu'}, a_+) g(\tilde{\lambda} + \frac{i\pi}{\mu'}, a_-) \quad (7.39)$$

hence giving the following for each boundary's scattering amplitude (up to a rapidity-independant phase factor),

$$\beta(\tilde{\lambda}, a_\pm) = S_0(\tilde{\lambda}) S_1(\tilde{\lambda}, a_\pm) g(\tilde{\lambda} + \frac{i\pi}{\mu'}, a_\pm) \quad (7.40)$$

7.3.3 Relation to boundary sine-Gordon model

Next, we briefly review Ghoshal-Zamolodchikov's results for the one boundary sine-Gordon theory [6]. We borrow conventions used in [43, 100]. Ghoshal-

[37] We are only able to use McCoy's method to exactly solve for the Bethe roots for systems up to only 6 sites due to computer limitations.

Zamolodchikov's results imply that the right and left boundary S matrices $R(\theta\,;\eta_\pm,\vartheta_\pm,\gamma_\pm)$ are given by

$$R(\theta\,;\eta,\vartheta,\gamma) = r_0(\theta)\ r_1(\theta\,;\eta,\vartheta)\ M(\theta\,;\eta,\vartheta,\gamma)\,, \tag{7.41}$$

where M has matrix elements

$$M(\theta\,;\eta,\vartheta,\gamma) = \left(\begin{array}{cc} m_{11} & m_{12} \\ m_{21} & m_{22} \end{array}\right)\,, \tag{7.42}$$

where $(\eta_\pm,\vartheta_\pm,\gamma_\pm)$ are the Ghoshal-Zamolodchikov's IR parameters and θ is the hole-rapidity. Further,

$$\begin{aligned}
m_{11} &= \cos\eta\cosh\vartheta\cosh(\tau\theta) + i\sin\eta\sinh\vartheta\sinh(\tau\theta)\,,\\
m_{22} &= \cos\eta\cosh\vartheta\cosh(\tau\theta) - i\sin\eta\sinh\vartheta\sinh(\tau\theta)\,,\\
m_{12} &= ie^{i\gamma}\sinh(\tau\theta)\cosh(\tau\theta)\,,\\
m_{21} &= ie^{-i\gamma}\sinh(\tau\theta)\cosh(\tau\theta)\,.
\end{aligned} \tag{7.43}$$

where $\tau = \frac{1}{\nu-1}$ is the bulk coupling constant. The scalar factors have the following integral representations [43, 100]

$$\begin{aligned}
r_0(\theta) &= \exp\left\{2i\int_0^\infty \frac{d\omega}{\omega}\sin(2\theta\omega/\pi)\frac{\sinh((\nu-2)\omega/2)\sinh(3\omega/2)}{\sinh((\nu-1)\omega/2)\sinh(2\omega)}\right\}\,,\\
r_1(\theta\,;\eta,\vartheta) &= \frac{1}{\cos\eta\cosh\vartheta}\sigma(\eta,\theta)\ \sigma(i\vartheta,\theta)\,,
\end{aligned} \tag{7.44}$$

where

$$\sigma(x,\theta) = \exp\left\{2\int_0^\infty \frac{d\omega}{\omega}\sin((i\pi-\theta)\omega/(2\pi))\sin(\theta\omega/(2\pi))\frac{\cosh((\nu-1)\omega x/\pi)}{\sinh((\nu-1)\omega/2)\cosh(\omega/2)}\right\}\,. \tag{7.45}$$

Our result (7.33) and (7.39) agree with the eigenvalues of $R(\theta\,;\eta_+,\vartheta_+,\gamma_+)R(\theta\,;\eta_-,\vartheta_-,\gamma_-)$, provided we make the following identification,

$$\begin{aligned}
\eta_\pm &= \frac{\mu'}{2}(\nu-2a_\pm)\\
\theta &= \pi\tilde{\lambda}
\end{aligned} \tag{7.46}$$

In addition to (7.46), one should also take $\vartheta_\pm = \gamma_\pm = 0$, since they are related to the lattice parameters that appear in the spin chain Hamiltonian, (2.1) which have been set to zero. The same expression is given in [43] for the corresponding open XXZ spin chain with nondiagonal boundary terms but with a constraint among the boundary parameters, hence suggesting that (7.46) holds true in general. As noted above, the eigenvalues, (7.34) and (7.40) agree with the sine-Gordon boundary S matrix eigenvalues. Hence the two eigenvalues can be related as follows,

$$\frac{\alpha(\tilde{\lambda}, a_\pm)}{\beta(\tilde{\lambda}, a_\pm)} = \frac{\cosh(\frac{i\mu'}{2}(\nu - 2a_\pm)) + i\sinh(\mu'\tilde{\lambda})}{\cosh(\frac{i\mu'}{2}(\nu - 2a_\pm)) - i\sinh(\mu'\tilde{\lambda})} \tag{7.47}$$

Based on a recently proposed Bethe ansatz solution for an open spin-1/2 XXZ spin chain with nondiagonal boundary terms, we have derived the boundary scattering amplitude (equation (7.34)) for a certain one-hole state. We used a conjectured relation between the extra roots and the hole rapidity, namely (7.31), which we verified numerically. This result agrees with the corresponding S matrix result for the one boundary sine-Gordon model derived by Ghoshal and Zamolodchikov [6], provided the lattice and IR parameters are related according to (7.46). We obtained the second eigenvalue (7.40) by considering an independent one-hole state with a 2-string. This scattering amplitude (7.40), derived for the one-hole state with 2-string also agrees with Ghoshal-Zamolodchikov's result following conjecture (7.38), which we verified numerically and identification (7.46). It would be interesting to derive (7.31) and (7.38) analytically.

It will also be interesting to study the excitations for the more general case of the open XXZ spin chain, namely with six arbitrary boundary parameters and arbitrary anisotropy parameter, and derive its corresponding S matrix. Solutions (spectrums) have been proposed for the general case, using the representation theory of q-Onsager algebra [30] and the algebraic-functional method [31]. However, Bethe Ansatz solution for this general case has not been found so far although such a solution has been proposed lately for the XXZ spin chain with six boundary parameters at roots of unity [60]. In addition to the bulk excitations, one can equally well look at boundary excitations although this can be rather challenging even for the simpler case of spin chains with diagonal boundary terms [101].

Appendix 1

Here we briefly review the solution [27, 28] for the case that the constraint (2.3) is satisfied, in order to facilitate comparison with the new cases considered in text. The matrix $\mathcal{M}$ is then given by

$$\mathcal{M} = \begin{pmatrix} \Lambda(u) & -h(-u-\eta) & 0 & \ldots & 0 & -h(u) \\ -h(u+\eta) & \Lambda(u+\eta) & -h(-u-2\eta) & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -h(-u-(p+1)\eta) & 0 & 0 & \ldots & -h(u+p\eta) & \Lambda(u+p\eta) \end{pmatrix} \tag{A1.1}$$

where $h(u)$ must satisfy

$$h(u+i\pi) = h\left(u+(p+1)\eta\right) = h(u)\,, \tag{A1.2}$$

$$h(u+\eta)\ h(-u-\eta) = \delta(u)\,, \tag{A1.3}$$

$$\prod_{j=0}^{p} h(u+j\eta) + \prod_{j=0}^{p} h(-u-j\eta) = f(u)\,. \tag{A1.4}$$

A pair of solutions is given by $h(u) = h^{(\pm)}(u) = h_0(u) h_1^{(\pm)}(u)$ with $h_0(u)$ given by (3.23), and $h_1^{(\pm)}(u)$ given by

$$h_1^{(\pm)}(u) = (-1)^{N+1} 4 \sinh(u \pm \alpha_-) \cosh(u \pm \beta_-) \sinh(u \pm \alpha_+) \cosh(u \pm \beta_+) \tag{A1.5}$$

Indeed, $h_0(u)$ satisfies

$$\begin{aligned} h_0(u+\eta)\ h_0(-u-\eta) &= \delta_0(u)\,, \\ \prod_{j=0}^{p} h_0(u+j\eta) = \prod_{j=0}^{p} h_0(-u-j\eta) &= f_0(u)\,, \end{aligned} \tag{A1.6}$$

where $\delta_0(u)$ is given by (2.18), and $f_0(u)$ is given by (2.21) and (2.23) for p even and odd, respectively. Moreover, $h_1^{(\pm)}(u)$ satisfies

$$h_1^{(\pm)}(u+\eta)\ h_1^{(\pm)}(-u-\eta) = \delta_1(u)\,, \tag{A1.7}$$

where $\delta_1(u)$ is given by (2.19); and

$$\prod_{j=0}^{p} h_1^{(\pm)}(u+j\eta) + \prod_{j=0}^{p} h_1^{(\pm)}(-u-j\eta) = f_1(u) - (-1)^{p(N+1)} 2^{1-2p} \sinh^2\left(2(p+1)u\right)$$
$$\times \left[(-1)^N \cosh\left((p+1)(\alpha_- + \alpha_+ + \beta_- + \beta_+)\right) + \cosh\left((p+1)(\theta_- - \theta_+)\right)\right], \tag{A1.8}$$

where $f_1(u)$ is given by (2.22) and (2.24) for p even and odd, respectively. Hence, if the constraint (2.3) is satisfied, then the RHS of (A1.8) reduces to $f_1(u)$; hence, all the conditions (A1.2)-(A1.4) are fulfilled. The corresponding expression for the transfer matrix eigenvalues is given by

$$\Lambda^{(\pm)}(u) = h^{(\pm)}(u) \frac{Q^{(\pm)}(u-\eta)}{Q^{(\pm)}(u)} + h^{(\pm)}(-u-\eta) \frac{Q^{(\pm)}(u+\eta)}{Q^{(\pm)}(u)}, \tag{A1.9}$$

with

$$Q^{(\pm)}(u) = \prod_{j=1}^{M^{(\pm)}} \sinh(u - u_j^{(\pm)}) \sinh(u + u_j^{(\pm)} + \eta),$$
$$M^{(\pm)} = \frac{1}{2}(N - 1 \pm k), \tag{A1.10}$$

and Bethe Ansatz equations

$$\frac{h^{(\pm)}(u_j^{(\pm)})}{h^{(\pm)}(-u_j^{(\pm)} - \eta)} = -\frac{Q^{(\pm)}(u_j^{(\pm)} + \eta)}{Q^{(\pm)}(u_j^{(\pm)} - \eta)}, \qquad j = 1, \ldots, M^{(\pm)}. \tag{A1.11}$$

Appendix 2

The coefficients μ_k appearing in the function $Y(u)$ (5.13) are given as follows. For p even,

$$\begin{aligned}
\mu_0 &= 2^{-4p}\Big\{ -1 - \cosh^2((p+1)(\theta_- - \theta_+)) \\
&- \cosh(2(p+1)\alpha_-)\cosh(2(p+1)\alpha_+) + \cosh(2(p+1)\alpha_-)\cosh(2(p+1)\beta_-) \\
&+ \cosh(2(p+1)\alpha_+)\cosh(2(p+1)\beta_-) + \cosh(2(p+1)\alpha_-)\cosh(2(p+1)\beta_+) \\
&+ \cosh(2(p+1)\alpha_+)\cosh(2(p+1)\beta_+) - \cosh(2(p+1)\beta_-)\cosh(2(p+1)\beta_+) \\
&+ \Big[\cosh((p+1)(\alpha_- + \alpha_+))\cosh((p+1)(\beta_- - \beta_+)) \\
&- \cosh((p+1)(\alpha_- - \alpha_+))\cosh((p+1)(\beta_- + \beta_+))\Big]^2 \\
&+ 2(-1)^N\cosh((p+1)(\theta_- - \theta_+))\Big[\cosh((p+1)(\alpha_- - \alpha_+))\cosh((p+1)(\beta_- - \beta_+)) \\
&- \cosh((p+1)(\alpha_- + \alpha_+))\cosh((p+1)(\beta_- + \beta_+))\Big]\Big\}, \\
\mu_1 &= 2^{1-4p}\Big\{\cosh((p+1)(\alpha_- - \alpha_+))\Big[\cosh((p+1)(\alpha_- + \alpha_+)) \\
&+ (-1)^N\cosh((p+1)(\beta_- + \beta_+))\cosh((p+1)(\theta_- - \theta_+))\Big] \\
&- \cosh((p+1)(\beta_- - \beta_+))\Big[\cosh((p+1)(\beta_- + \beta_+)) \\
&+ (-1)^N\cosh((p+1)(\alpha_- + \alpha_+))\cosh((p+1)(\theta_- - \theta_+))\Big]\Big\}, \\
\mu_2 &= 2^{-4p}\sinh^2((p+1)(\theta_- - \theta_+)) \,. \qquad \text{(A2.1)}
\end{aligned}$$

For p odd,

$$\begin{aligned}
\mu_0 &= 2^{-4p}\Big\{ -1 - \cosh^2((p+1)(\theta_- - \theta_+)) \\
&- \cosh(2(p+1)\alpha_-)\cosh(2(p+1)\alpha_+) - \cosh(2(p+1)\alpha_-)\cosh(2(p+1)\beta_-) \\
&- \cosh(2(p+1)\alpha_+)\cosh(2(p+1)\beta_-) - \cosh(2(p+1)\alpha_-)\cosh(2(p+1)\beta_+)
\end{aligned}$$

$$
\begin{aligned}
&- \cosh(2(p+1)\alpha_+)\cosh(2(p+1)\beta_+) - \cosh(2(p+1)\beta_-)\cosh(2(p+1)\beta_+) \\
&+ \Big[\cosh((p+1)(\alpha_- + \alpha_+))\cosh((p+1)(\beta_- - \beta_+)) \\
&+ \cosh((p+1)(\alpha_- - \alpha_+))\cosh((p+1)(\beta_- + \beta_+))\Big]^2 \\
&- 2(-1)^N \cosh((p+1)(\theta_- - \theta_+))\Big[\cosh((p+1)(\alpha_- - \alpha_+))\cosh((p+1)(\beta_- - \beta_+)) \\
&+ \cosh((p+1)(\alpha_- + \alpha_+))\cosh((p+1)(\beta_- + \beta_+))\Big]\Big\}, \\
\mu_1 &= 2^{1-4p}\Big\{\cosh((p+1)(\alpha_- + \alpha_+))\Big[\cosh((p+1)(\alpha_- - \alpha_+)) \\
&+ (-1)^N \cosh((p+1)(\beta_- - \beta_+))\cosh((p+1)(\theta_- - \theta_+))\Big] \\
&+ \cosh((p+1)(\beta_- + \beta_+))\Big[\cosh((p+1)(\beta_- - \beta_+)) \\
&+ (-1)^N \cosh((p+1)(\alpha_- - \alpha_+))\cosh((p+1)(\theta_- - \theta_+))\Big]\Big\}, \\
\mu_2 &= 2^{-4p}\sinh^2((p+1)(\theta_- - \theta_+)) . \qquad \text{(A2.2)}
\end{aligned}
$$

The modified function $f(u)$ for the case $\eta = i\pi p/(p+1)$, with p a positive integer

$$
\begin{aligned}
f_0(u) &= (-1)^N 2^{-2pN} \sinh^{2N}((p+1)u) , \\
f_1(u) &= (-1)^N 2^{3-2p}\Big(\\
&- \sinh((p+1)\alpha_-)\cosh((p+1)\beta_-)\sinh((p+1)\alpha_+)\cosh((p+1)\beta_+)\cosh^2((p+1)u) \\
&+ \cosh((p+1)\alpha_-)\sinh((p+1)\beta_-)\cosh((p+1)\alpha_+)\sinh((p+1)\beta_+)\sinh^2((p+1)u) \\
&- \cosh((p+1)(\theta_- - \theta_+))\sinh^2((p+1)u)\cosh^2((p+1)u)\Big) . \qquad \text{(A2.3)}
\end{aligned}
$$

Correspondingly, the coefficients μ_0 and μ_1 are given by (A2.1) with the factor $(-1)^N$ replaced by -1. Apart from these changes, the solution is the same as for the case (2.70) for both odd and even p.

Appendix 3

Here we present more explicit expressions for the bulk and boundary energies.

3.0.4 Case I: p even

The integral appearing in the bulk energy (5.41) for p even is given by

$$\begin{aligned} I_1 &\equiv \int_{-\infty}^{\infty} d\lambda\ a_1(\lambda)\ s(\lambda) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\ \hat{a}_1(\omega)\ \hat{s}(\omega) \\ &= \frac{\mu}{\pi}\sum_{j=1}^{\frac{p}{2}}(-1)^{j+\frac{p}{2}} \tan\Big((j-\frac{1}{2})\mu\Big)\,. \end{aligned} \tag{A3.1}$$

The parameter-dependent integral appearing in the boundary energy (4.38) is given by

$$\begin{aligned} I_2(x) &\equiv \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\ \frac{\sinh(\omega/2)\cos(x\omega)}{2\sinh(\nu\omega/2)\cosh(\omega/2)} \\ &= \sum_{j=1}^{\frac{p}{2}}(-1)^{j+\frac{p}{2}} b_{j-\frac{1}{2}}(x/2) - \frac{1}{2} b_{\frac{p+1}{2}}(x/2)\,, \end{aligned} \tag{A3.2}$$

where the function $b_n(\lambda)$ is defined in (4.26). Moreover,

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\ \frac{\sinh(\omega/2)\cosh((\nu-2)\omega/2)}{2\sinh(\nu\omega/2)\cosh(\omega/2)} = I_2(i(p-1)/2)\,, \tag{A3.3}$$

and

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\ \frac{\sinh((\nu-2)\omega/4)}{4\sinh(\nu\omega/4)\cosh(\omega/2)} = \frac{1}{2}\left[I_1 - I_2(0)\right]\,. \tag{A3.4}$$

It follows that the boundary energy (4.38) is given by

$$E^{\pm}_{boundary} = -\frac{\pi\sin\mu}{\mu}\Big\{\frac{1}{2}I_1 - \frac{1}{2}I_2(0) + I_2(i(p-1)/2) + I_2(b_\pm) - \frac{1}{4}\Big\} - \frac{1}{4}\cos\mu\,, \tag{A3.5}$$

where I_1 and $I_2(x)$ are given by (A3.1) and (A3.2), respectively.

3.0.5 Case II: p odd

The integral appearing in the bulk energy (5.41) for p odd is given by

$$\begin{aligned} I_1 &\equiv \int_{-\infty}^{\infty} d\lambda\ a_1(\lambda)\ s(\lambda) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega\ \hat{a}_1(\omega)\ \hat{s}(\omega) \\ &= \frac{\mu}{\pi^2} \Big[1 + 2\mu \sum_{j=1}^{\frac{p-1}{2}} j \cot(j\mu) \Big] . \end{aligned} \tag{A3.6}$$

The parameter-dependent integral appearing in the boundary energy (4.66) is given by

$$\begin{aligned} I_2(x) &\equiv \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega\ \frac{\sinh(\omega/2)\cosh(x\omega)}{2\sinh(\nu\omega/2)\cosh(\omega/2)} \\ &= \frac{(-1)^{\frac{p-1}{2}}\mu}{\pi \sin(x\pi)} \left[x + \sum_{j=1}^{\frac{p-1}{2}} (-1)^j \cot(j\mu) \sin(2xj\mu) \right] . \end{aligned} \tag{A3.7}$$

Moreover,

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega\ \frac{\cosh((\nu-2)\omega/4)}{4\cosh(\nu\omega/4)\cosh(\omega/2)} = \frac{1}{2} \left[I_1 + I_2(0) \right] . \tag{A3.8}$$

It follows that the boundary energy (4.66) is given by

$$E^{\pm}_{boundary} = -\frac{\pi \sin\mu}{\mu} \Big\{ \frac{1}{2} I_1 + \frac{1}{2} I_2(0) + I_2((p+1-2|a_\pm|)/2) - \frac{1}{4} \Big\} - \frac{1}{4} \cos\mu , \tag{A3.9}$$

where I_1 and $I_2(x)$ are given by (A3.6) and (A3.7), respectively.

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