

Boundary energy of the general open XXZ chain at roots of unity

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ABSTRACT: We have recently proposed a Bethe Ansatz solution of the open spin-1/2 XXZ quantum spin chain with general integrable boundary terms (containing six free boundary parameters) at roots of unity. We use this solution, together with an appropriate string hypothesis, to compute the boundary energy of the chain in the thermodynamic limit.

KEYWORDS: Bethe Ansatz, Lattice Integrable Models, Boundary Quantum Field Theory.

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1. Introduction

There has been considerable interest in the open spin-1/2 XXZ quantum spin chain with general integrable boundary terms [1, 2], whose Hamiltonian can be written as

$$\begin{aligned}
 \mathcal{H} = & \frac{1}{2} \sum_{n=1}^{N-1} (\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \cosh \eta \sigma_n^z \sigma_{n+1}^z) \\
 & + \frac{1}{2} \sinh \eta \left[\coth \alpha_- \tanh \beta_- \sigma_1^z + \operatorname{cosech} \alpha_- \operatorname{sech} \beta_- (\cosh \theta_- \sigma_1^x + i \sinh \theta_- \sigma_1^y) \right. \\
 & \left. - \coth \alpha_+ \tanh \beta_+ \sigma_N^z + \operatorname{cosech} \alpha_+ \operatorname{sech} \beta_+ (\cosh \theta_+ \sigma_N^x + i \sinh \theta_+ \sigma_N^y) \right], \quad (1.1)
 \end{aligned}$$

where η is the bulk anisotropy parameter, and $\alpha_{\pm}, \beta_{\pm}, \theta_{\pm}$ are free boundary parameters.¹

Except for the special case α_{\pm} or $\beta_{\pm} \rightarrow \infty$ when the boundary terms become diagonal [3–5], the boundary terms break the bulk $U(1)$ symmetry generated by S^z ; i.e., the model has no continuous symmetry. For generic values of boundary parameters, this model does not seem to have a simple pseudovacuum, which precludes constructing a

¹Under a global spin rotation about the z axis, the bulk terms remain invariant, and the boundary parameters θ_{\pm} become shifted by the same constant, $\theta_{\pm} \mapsto \theta_{\pm} + \text{const}$. Hence, the energy (and in fact, the transfer matrix eigenvalues) depend on θ_{\pm} only through the difference $\theta_- - \theta_+$.

conventional algebraic Bethe Ansatz solution. Being associated with the spin-1/2 representation of $U_q(su(2))$, this model is but the simplest of an infinite hierarchy of more complicated integrable quantum spin chains involving higher-dimensional representations and/or higher-rank algebras. Hence, solving the former model is presumably a prerequisite for solving any of the latter ones. This model also has numerous applications in statistical mechanics, condensed matter and quantum field theory.

A Bethe Ansatz solution of this model was found in [6–9] for the case that the boundary parameters obey the constraint

$$\alpha_- + \epsilon_1\beta_- + \epsilon_2\alpha_+ + \epsilon_3\beta_+ = \epsilon_0(\theta_- - \theta_+) + \eta k + \frac{1 - \epsilon_2}{2}i\pi \pmod{2i\pi}, \quad \epsilon_1\epsilon_2\epsilon_3 = +1, \quad (1.2)$$

where $\epsilon_i = \pm 1$, and k is an integer such that $|k| \leq N-1$ and $N-1+k$ is even. 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 [8]. Related work includes [10–16].

There remained the problem of solving the model (1.1) when the constraint (1.2) is *not* satisfied. Building on earlier work [17, 18], we recently proposed in [19] a solution of the model for arbitrary values of the boundary parameters, provided that the bulk anisotropy parameter has values

$$\eta = \frac{i\pi}{p+1}, \quad (1.3)$$

where p is a positive integer. Hence, $q \equiv e^\eta$ is a root of unity, satisfying $q^{p+1} = -1$.

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 [19], 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 [18] for special values of the boundary parameters.)

The solution [19] 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 ($N \rightarrow \infty$) 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 [4], and then analytically in [20].

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 (3.28) for the boundary energy coincides with the result obtained in [21] for the case that the boundary parameters obey the constraint (1.2), and in [22] for special values [17, 18] of the boundary parameters at roots of unity.

The outline of this paper is as follows. In section 2, we briefly review the Bethe Ansatz solution [19] of the model (1.1) at roots of unity (1.3). In section 3, we treat the case of even p , followed by the case of odd p in section 4. This is followed by discussion of our results and a brief outline of our future work in section 5.

2. Bethe Ansatz

In this section, we briefly recall the Bethe Ansatz solution [19]. In order to ensure hermiticity of the Hamiltonian (1.1), we take the boundary parameters β_{\pm} real; α_{\pm} imaginary; θ_{\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 $b_j(u)$:

$$a_j(u) = A_j \prod_{k=1}^{2M_a} \sinh(u - u_k^{(a_j)}), \quad b_j(u) = B_j \prod_{k=1}^{2M_b} \sinh(u - u_k^{(b_j)}),$$

$$j = 1, \dots, \lfloor \frac{p+1}{2} \rfloor, \tag{2.1}$$

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

$$a_{\frac{p}{2}+1}(u) = A_{\frac{p}{2}+1} \prod_{k=1}^{M_a} \sinh(u - u_k^{(a_{\frac{p}{2}+1})}) \sinh(u + u_k^{(a_{\frac{p}{2}+1})}),$$

$$b_{\frac{p}{2}+1}(u) = B_{\frac{p}{2}+1} \prod_{k=1}^{M_b} \sinh(u - u_k^{(b_{\frac{p}{2}+1})}) \sinh(u + u_k^{(b_{\frac{p}{2}+1})}). \tag{2.2}$$

The normalization constants $\{A_j, B_j\}$ are yet to be determined.² We assume that N is even, in which case the integers M_a, M_b are given by

$$M_a = \frac{N}{2} + 2p, \quad M_b = \frac{N}{2} + p - 1, \tag{2.3}$$

It is clear from (2.1), (2.2) that $a_j(u)$ and $b_j(u)$ have the following periodicity and crossing properties,

$$a_j(u + i\pi) = a_j(u), \quad b_j(u + i\pi) = b_j(u), \quad j = 1, \dots, \lfloor \frac{p}{2} \rfloor + 1, \tag{2.4}$$

$$a_{\frac{p}{2}+1}(-u) = a_{\frac{p}{2}+1}(u), \quad b_{\frac{p}{2}+1}(-u) = b_{\frac{p}{2}+1}(u). \tag{2.5}$$

²One of these normalization constants can be set to unity.

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

$$\frac{h_0(-u_l^{(a_1)} - \eta)}{h_0(u_l^{(a_1)})} = -\frac{f_1(u_l^{(a_1)}) a_1(-u_l^{(a_1)}) + g_1(u_l^{(a_1)}) Y(u_l^{(a_1)})^2 b_1(-u_l^{(a_1)})}{2a_2(u_l^{(a_1)}) h_1(-u_l^{(a_1)} - \eta) \prod_{k=1}^p h_1(u_l^{(a_1)} + k\eta)}, \quad (2.6)$$

$$\frac{h(-u_l^{(a_j)} - j\eta)}{h(u_l^{(a_j)} + (j-1)\eta)} = -\frac{a_{j-1}(u_l^{(a_j)})}{a_{j+1}(u_l^{(a_j)})}, \quad j = 2, \dots, \lfloor \frac{p}{2} \rfloor + 1, \quad (2.7)$$

and

$$\frac{h_0(-u_l^{(b_1)} - \eta)}{h_0(u_l^{(b_1)})} = -\frac{f_1(u_l^{(b_1)}) b_1(-u_l^{(b_1)}) + g_1(u_l^{(b_1)}) a_1(-u_l^{(b_1)})}{2b_2(u_l^{(b_1)}) h_1(-u_l^{(b_1)} - \eta) \prod_{k=1}^p h_1(u_l^{(b_1)} + k\eta)}, \quad (2.8)$$

$$\frac{h(-u_l^{(b_j)} - j\eta)}{h(u_l^{(b_j)} + (j-1)\eta)} = -\frac{b_{j-1}(u_l^{(b_j)})}{b_{j+1}(u_l^{(b_j)})}, \quad j = 2, \dots, \lfloor \frac{p}{2} \rfloor + 1, \quad (2.9)$$

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,

$$h(u) = h_0(u) h_1(u), \quad (2.10)$$

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

$$\begin{aligned} h_0(u) &= \sinh^{2N}(u + \eta) \frac{\sinh(2u + 2\eta)}{\sinh(2u + \eta)}, \\ h_1(u) &= -4 \sinh(u + \alpha_-) \cosh(u + \beta_-) \sinh(u + \alpha_+) \cosh(u + \beta_+). \end{aligned} \quad (2.11)$$

We also define the quantities

$$g_1(u) = 2 \sinh(2(p+1)u) \quad (2.12)$$

and

$$Y(u)^2 = \sum_{k=0}^2 \mu_k \cosh^k(2(p+1)u). \quad (2.13)$$

Explicit expressions for the coefficients μ_k in (2.13), which depend on the boundary parameters, as well as for the function $f_1(u)$, are listed in the appendix for both even and odd values of p .

Moreover, there are additional Bethe- Ansatz-like equations

$$a_1\left(\frac{\eta}{2}\right) = a_2\left(-\frac{\eta}{2}\right), \quad (2.14)$$

$$a_{j-1}\left(\left(\frac{1}{2} - j\right)\eta\right) = a_{j+1}\left(\left(\frac{1}{2} - j\right)\eta\right), \quad j = 2, \dots, \lfloor \frac{p}{2} \rfloor + 1, \quad (2.15)$$

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

$$b_1\left(\frac{\eta}{2}\right) = b_2\left(-\frac{\eta}{2}\right), \quad (2.16)$$

$$b_{j-1}\left(\left(\frac{1}{2} - j\right)\eta\right) = b_{j+1}\left(\left(\frac{1}{2} - j\right)\eta\right), \quad j = 2, \dots, \lfloor \frac{p}{2} \rfloor + 1, \quad (2.17)$$

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

$$f_1(-\alpha_- - \eta) b_1(\alpha_- + \eta) = -g_1(-\alpha_- - \eta) a_1(\alpha_- + \eta). \quad (2.18)$$

The energy eigenvalues of the Hamiltonian (1.1) are given by

$$E = \frac{1}{2} \sinh \eta \sum_{l=1}^{2M_b} \left[\coth(u_l^{(b_j)} + (j-1)\eta) - \coth(u_l^{(b_{j-1})} + (j-1)\eta) \right] + E_0, \\ j = 2, \dots, \lfloor \frac{p+1}{2} \rfloor, \quad (2.19)$$

where E_0 is defined as

$$E_0 = \frac{1}{2} \sinh \eta (\coth \alpha_- + \tanh \beta_- + \coth \alpha_+ + \tanh \beta_+) + \frac{1}{2} (N-1) \cosh \eta. \quad (2.20)$$

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

$$E = \frac{1}{2} \sinh \eta \left\{ \sum_{l=1}^{M_b} \left[\coth(u_l^{(b_{\frac{p}{2}+1})} + \frac{p\eta}{2}) - \coth(u_l^{(b_{\frac{p}{2}+1})} - \frac{p\eta}{2}) \right] - \sum_{l=1}^{2M_b} \coth(u_l^{(b_{\frac{p}{2}})} + \frac{p\eta}{2}) \right\} + E_0. \quad (2.21)$$

There are also similar expressions for the energy in terms of a roots $\{u_l^{(a_j)}\}$ [19].

3. Even p

In this section, we consider the case where the bulk anisotropy parameter assumes the values (1.3) with p even, i.e., $\eta = \frac{i\pi}{3}, \frac{i\pi}{5}, \dots$. We have studied the Bethe roots corresponding to the ground state numerically for small values of p and N along the lines of [8]. We have found that, when the boundary parameters are in some suitable domain (which we discuss further below eq. (3.28)), 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 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”.

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 any even p are summarized below,

$$v_k^{\pm(a_j)} = v_k^{\pm(b_j)} = \pm \tilde{v}_k + \left(\frac{2p+3-2j}{2} \right) \eta, \quad k = 1, \dots, \frac{N}{2}, \\ j = 1, \dots, \frac{p}{2} + 1, \quad (3.1)$$

where \tilde{v}_k are real and positive. In figure 1, the sea roots are indicated with red stars.

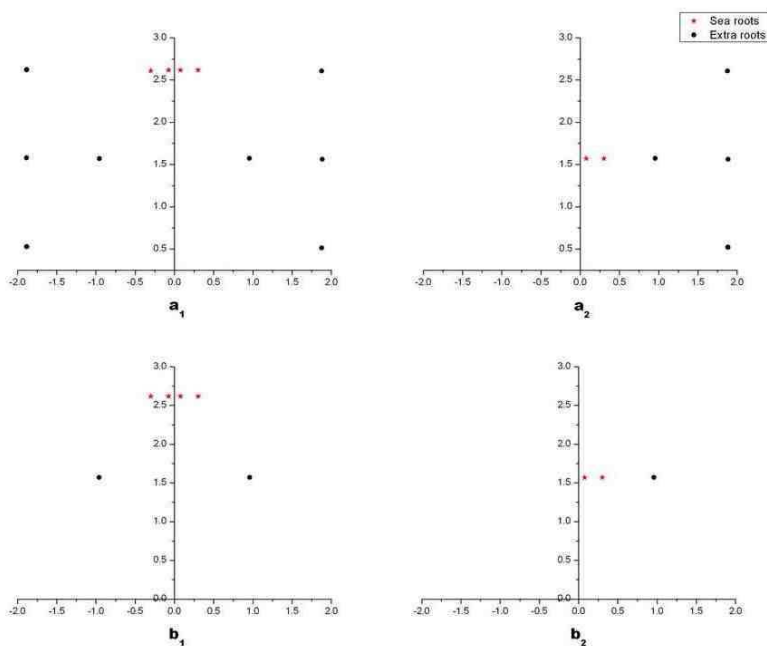


Figure 1: Ground-state Bethe roots for $p = 2$, $N = 4$, $\alpha_- = 0.604i$, $\alpha_+ = 0.535i$, $\beta_- = -1.882$, $\beta_+ = 1.878$, $\theta_- = 0.6i$, $\theta_+ = 0.7i$.

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 (2.5) of the functions $a_{\frac{p}{2}+1}(u)$ and $b_{\frac{p}{2}+1}(u)$.³

3.2 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 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

$$w_k^{\pm(b_j)} = \pm\tilde{w}_k + \left(\frac{2p+1-2k}{2}\right)\eta, \quad k = 1, \dots, p-1, \\ j = 1, \dots, \frac{p}{2} + 1. \tag{3.2}$$

³Hence, strictly speaking, we should write the $j = \frac{p}{2} + 1$ equation in (3.1) 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,

$$\tilde{w}_k = \tilde{w}_{p-k}, \quad k = 1, \dots, \frac{p}{2} - 1. \quad (3.3)$$

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:

$$\begin{aligned} w_k^{\pm(a_j,1)} &= w_k^{\pm(b_j)} = \pm \tilde{w}_k + \left(\frac{2p+1-2k}{2} \right) \eta, \quad k = 1, \dots, p-1, \\ w_k^{\pm(a_j,2)} &= \pm \tilde{w}_0 + \left(\frac{2p+3-2k}{2} \right) \eta, \quad k = 1, \dots, p+1, \\ & j = 1, \dots, \frac{p}{2} + 1. \end{aligned} \quad (3.4)$$

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.

3.3 Boundary energy

We now proceed to compute the boundary energy. Using the expression (2.19) for the energy and our string hypothesis, we obtain (for $p > 2$)

$$\begin{aligned} E &= \frac{1}{2} \sinh \eta \left\{ \sum_{k=1}^{\frac{N}{2}} \left[\coth(v_k^{+(b_j)} + (j-1)\eta) + \coth(v_k^{-(b_j)} + (j-1)\eta) \right. \right. \\ &\quad \left. \left. - \coth(v_k^{+(b_{j-1})} + (j-1)\eta) - \coth(v_k^{-(b_{j-1})} + (j-1)\eta) \right] \right. \\ &\quad \left. + \sum_{k=1}^{p-1} \left[\coth(w_k^{+(b_j)} + (j-1)\eta) + \coth(w_k^{-(b_j)} + (j-1)\eta) \right. \right. \\ &\quad \left. \left. - \coth(w_k^{+(b_{j-1})} + (j-1)\eta) - \coth(w_k^{-(b_{j-1})} + (j-1)\eta) \right] \right\} + E_0, \\ & j = 2, \dots, \frac{p}{2}. \end{aligned} \quad (3.5)$$

Recalling (3.1) and (3.2), this expression for the energy reduces to

$$E = \sinh^2 \eta \sum_{k=1}^{\frac{N}{2}} \frac{1}{\sinh(\tilde{v}_k - \frac{\eta}{2}) \sinh(\tilde{v}_k + \frac{\eta}{2})} + E_0, \quad \tilde{v}_k > 0, \quad (3.6)$$

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 (3.6). The same result can also be obtained (for $p \geq 2$) from the energy expression (2.21).

We turn now to the Bethe Ansatz equations, on which we must also impose our string hypothesis. Choosing $j = \frac{p}{2} + 1$ in (2.9) 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

$$\frac{h(-\tilde{v}_l - \frac{\eta}{2})}{h(\tilde{v}_l - \frac{\eta}{2})} = -\frac{b_{\frac{p}{2}}(\tilde{v}_l + \frac{i\pi}{2})}{b_{\frac{p}{2}}(-\tilde{v}_l - \frac{i\pi}{2})}, \quad (3.7)$$

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

$$\begin{aligned} & \left(\frac{\sinh(\tilde{v}_l + \frac{\eta}{2})}{\sinh(\tilde{v}_l - \frac{\eta}{2})} \right)^{2N} \frac{\sinh(2\tilde{v}_l + \eta) \sinh(\tilde{v}_l - \frac{\eta}{2} + \alpha_-) \cosh(\tilde{v}_l - \frac{\eta}{2} + \beta_-)}{\sinh(2\tilde{v}_l - \eta) \sinh(\tilde{v}_l + \frac{\eta}{2} - \alpha_-) \cosh(\tilde{v}_l + \frac{\eta}{2} - \beta_-)} \\ & \times \frac{\sinh(\tilde{v}_l - \frac{\eta}{2} + \alpha_+) \cosh(\tilde{v}_l - \frac{\eta}{2} + \beta_+)}{\sinh(\tilde{v}_l + \frac{\eta}{2} - \alpha_+) \cosh(\tilde{v}_l + \frac{\eta}{2} - \beta_+)} = - \prod_{k=1}^{\frac{N}{2}} \frac{\sinh(\tilde{v}_l - \tilde{v}_k + \eta) \sinh(\tilde{v}_l + \tilde{v}_k + \eta)}{\sinh(\tilde{v}_l - \tilde{v}_k - \eta) \sinh(\tilde{v}_l + \tilde{v}_k - \eta)}, \\ & l = 1, \dots, \frac{N}{2}, \quad \tilde{v}_k > 0. \end{aligned} \quad (3.8)$$

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 r.h.s. cancel as a consequence of the relation (3.3) among their real parts.

Remarkably, as a consequence of our string hypothesis, our non-conventional Bethe Ansatz equations have reduced to a conventional system (3.8), 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,

$$A_1 = A_2 = \dots = A_{\frac{p}{2}+1}, \quad B_1 = B_2 = \dots = B_{\frac{p}{2}+1}. \quad (3.9)$$

This result follows from the Bethe-Ansatz-like equations (2.14)–(2.17) and the string hypothesis. For example, using (3.1) and (3.2) in (2.16), and remembering the relation (3.3) among the real parts of the extra roots, we obtain $B_1 = B_2$. Hence, choosing $u_l^{(b_j)}$ in (2.9) to be a sea root $v_l^{+(b_j)}$ for any $j \in \{2, \dots, \frac{p}{2} + 1\}$, we again arrive at (3.8). Moreover, in view of the identity

$$\frac{a_{j-1}(v_l^{+(a_j)})}{a_{j+1}(v_l^{+(a_j)})} = \frac{b_{j-1}(v_l^{+(b_j)})}{b_{j+1}(v_l^{+(b_j)})}, \quad j = 2, \dots, \frac{p}{2} + 1, \quad (3.10)$$

where $v_l^{+(a_j)} = v_l^{+(b_j)}$ is a sea root, the same result (3.8) can also be obtained from (2.7).⁴

In the thermodynamic ($N \rightarrow \infty$) 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. To this end, following [21, 22] and references therein, we define some basic quantities

$$e_n(\lambda) = \frac{\sinh \mu \left(\lambda + \frac{i\eta}{2} \right)}{\sinh \mu \left(\lambda - \frac{i\eta}{2} \right)}, \quad g_n(\lambda) = e_n(\lambda \pm \frac{i\pi}{2\mu}) = \frac{\cosh \mu \left(\lambda + \frac{i\eta}{2} \right)}{\cosh \mu \left(\lambda - \frac{i\eta}{2} \right)}, \quad (3.11)$$

⁴Only the first set of Bethe equations (2.6), (2.8) do not seem to reduce to (3.8).

which allow us to rewrite the Bethe Ansatz equations (3.8) in a more compact form,

$$e_1(\lambda_l)^{2N+1} g_1(\lambda_l) \frac{e_{2a_- - 1}(\lambda_l) e_{2a_+ - 1}(\lambda_l)}{g_{1+2ib_-}(\lambda_l) g_{1+2ib_+}(\lambda_l)} = - \prod_{k=1}^{\frac{N}{2}} e_2(\lambda_l - \lambda_k) e_2(\lambda_l + \lambda_k),$$

$$l = 1, \dots, \frac{N}{2}, \quad (3.12)$$

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 (3.12), we obtain the desired ground state counting function

$$\mathbf{h}(\lambda) = \frac{1}{2\pi} \left\{ (2N+1)q_1(\lambda) + r_1(\lambda) + q_{2a_- - 1}(\lambda) - r_{1+2ib_-}(\lambda) + q_{2a_+ - 1}(\lambda) - r_{1+2ib_+}(\lambda) \right. \\ \left. - \sum_{k=1}^{\frac{N}{2}} [q_2(\lambda - \lambda_k) + q_2(\lambda + \lambda_k)] \right\}, \quad (3.13)$$

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

$$q_n(\lambda) = \pi + i \ln e_n(\lambda) = 2 \tan^{-1} (\cot(n\mu/2) \tanh(\mu\lambda)),$$

$$r_n(\lambda) = i \ln g_n(\lambda). \quad (3.14)$$

Defining $\lambda_{-k} \equiv -\lambda_k$, we have

$$- \sum_{k=1}^{\frac{N}{2}} [q_2(\lambda - \lambda_k) + q_2(\lambda + \lambda_k)] = - \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} q_2(\lambda - \lambda_k) + q_2(\lambda). \quad (3.15)$$

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

$$\rho(\lambda) = \frac{1}{N} \frac{d\mathbf{h}}{d\lambda} = 2a_1(\lambda) - \int_{-\infty}^{\infty} d\lambda' a_2(\lambda - \lambda') \rho(\lambda') + \frac{1}{N} [a_1(\lambda) + b_1(\lambda) \\ + a_2(\lambda) + a_{2a_- - 1}(\lambda) - b_{1+2ib_-}(\lambda) + a_{2a_+ - 1}(\lambda) - b_{1+2ib_+}(\lambda)], \quad (3.16)$$

where we have ignored corrections of higher order in $1/N$ when passing from a sum to an integral, and we have introduced the notations⁵

$$a_n(\lambda) = \frac{1}{2\pi} \frac{d}{d\lambda} q_n(\lambda) = \frac{\mu}{\pi} \frac{\sin(n\mu)}{\cosh(2\mu\lambda) - \cos(n\mu)},$$

$$b_n(\lambda) = \frac{1}{2\pi} \frac{d}{d\lambda} r_n(\lambda) = -\frac{\mu}{\pi} \frac{\sin(n\mu)}{\cosh(2\mu\lambda) + \cos(n\mu)}. \quad (3.17)$$

The solution of the linear integral equation (3.16) for $\rho(\lambda)$ is obtained by Fourier transforms and is given by⁶

$$\rho(\lambda) = 2s(\lambda) + \frac{1}{N} R(\lambda), \quad (3.18)$$

⁵These 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. We apologize for this unfortunate coincidence of notations.

⁶Our conventions are

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

where

$$s(\lambda) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega\lambda} \frac{1}{2 \cosh(\omega/2)} = \frac{1}{2 \cosh(\pi\lambda)}, \quad (3.19)$$

and

$$\hat{R}(\omega) = \frac{1}{(1 + \hat{a}_2(\omega))} \left\{ \hat{a}_1(\omega) + \hat{b}_1(\omega) + \hat{a}_2(\omega) - \hat{b}_{1+2ib_-}(\omega) - \hat{b}_{1+2ib_+}(\omega) \right. \\ \left. + \hat{a}_{2a_- - 1}(\omega) + \hat{a}_{2a_+ - 1}(\omega) \right\}, \quad (3.20)$$

with

$$\hat{a}_n(\omega) = \text{sgn}(n) \frac{\sinh((\nu - |n|)\omega/2)}{\sinh(\nu\omega/2)}, \quad 0 \leq |n| < 2\nu, \quad (3.21)$$

$$\hat{b}_n(\omega) = -\frac{\sinh(n\omega/2)}{\sinh(\nu\omega/2)}, \quad 0 < \Re n < \nu, \quad (3.22)$$

where $\nu \equiv \frac{\pi}{\mu} = p + 1$.

Expressing the energy expression (3.6) in terms of the newly defined quantities and letting N become large, we obtain

$$E = -\frac{2\pi \sin \mu}{\mu} \sum_{k=1}^{\frac{N}{2}} a_1(\lambda_k) + E_0 = -\frac{\pi \sin \mu}{\mu} \left\{ \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} a_1(\lambda_k) - a_1(0) \right\} + E_0 \\ = -\frac{\pi \sin \mu}{\mu} \left\{ N \int_{-\infty}^{\infty} d\lambda a_1(\lambda) \rho(\lambda) - a_1(0) \right\} + \frac{1}{2}(N-1) \cos \mu \\ + \frac{1}{2} \sin \mu (\cot \mu a_- + i \tanh \mu b_- + \cot \mu a_+ + i \tanh \mu b_+), \quad (3.23)$$

where again we ignore corrections that are higher order in $1/N$. Substituting the result (3.18) for the root density, we obtain

$$E = E_{\text{bulk}} + E_{\text{boundary}}, \quad (3.24)$$

where the bulk (order N) energy is given by

$$E_{\text{bulk}} = -\frac{2N\pi \sin \mu}{\mu} \int_{-\infty}^{\infty} d\lambda a_1(\lambda) s(\lambda) + \frac{1}{2}N \cos \mu \\ = -N \sin^2 \mu \int_{-\infty}^{\infty} d\lambda \frac{1}{[\cosh(2\mu\lambda) - \cos \mu] \cosh(\pi\lambda)} + \frac{1}{2}N \cos \mu, \quad (3.25)$$

which agrees with the well-known result [23]. The boundary (order 1) energy is given by

$$E_{\text{boundary}} = -\frac{\pi \sin \mu}{\mu} I - \frac{1}{2} \cos \mu + \frac{1}{2} \sin \mu (\cot \mu a_- + i \tanh \mu b_- + \cot \mu a_+ + i \tanh \mu b_+), \quad (3.26)$$

where I is the integral

$$I = \int_{-\infty}^{\infty} d\lambda a_1(\lambda) [R(\lambda) - \delta(\lambda)] = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \hat{a}_1(\omega) [\hat{R}(\omega) - 1] \\ = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \hat{s}(\omega) \left\{ \hat{a}_1(\omega) + \hat{b}_1(\omega) - 1 \right. \\ \left. - \hat{b}_{1+2ib_-}(\omega) - \hat{b}_{1+2ib_+}(\omega) + \hat{a}_{2a_- - 1}(\omega) + \hat{a}_{2a_+ - 1}(\omega) \right\}. \quad (3.27)$$

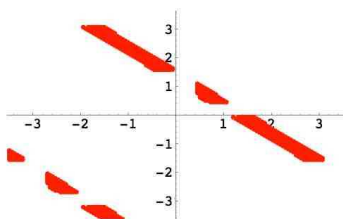


Figure 2: Shaded area denotes region of the $(\Im m \alpha_+, \Im m \alpha_-)$ plane for which the ground-state Bethe roots obey the string hypothesis for $p = 2$, $N = 2$, $\beta_- = -1.882$, $\beta_+ = 1.878$, $\theta_- = 0.6i$, $\theta_+ = 0.7i$.

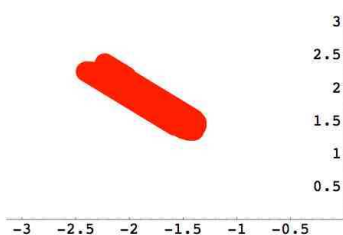


Figure 3: Shaded area denotes region of the (β_+, β_-) plane for which the ground-state Bethe roots obey the string hypothesis for $p = 2$, $N = 2$, $\alpha_- = -1.818i$, $\alpha_+ = 2.959i$, $\theta_- = 0.7i$, $\theta_+ = 0.6i$.

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

$$\begin{aligned}
 E_{\text{boundary}}^\pm &= -\frac{\sin \mu}{2\mu} \int_{-\infty}^{\infty} d\omega \frac{1}{2 \cosh(\omega/2)} \left\{ \frac{\sinh((\nu - 2)\omega/4)}{2 \sinh(\nu\omega/4)} - \frac{1}{2} \right. \\
 &\quad \left. + \operatorname{sgn}(2a_\pm - 1) \frac{\sinh((\nu - |2a_\pm - 1|)\omega/2)}{\sinh(\nu\omega/2)} + \frac{\sinh((2ib_\pm + 1)\omega/2)}{\sinh(\nu\omega/2)} \right\} \\
 &\quad + \frac{1}{2} \sin \mu (\cot \mu a_\pm + i \tanh \mu b_\pm) - \frac{1}{4} \cos \mu.
 \end{aligned} \tag{3.28}$$

This result can be shown to coincide with previous results in [21, 22].

We emphasize that the result (3.28) 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 2 and 3 denote regions of parameter space for which the ground-state Bethe roots have the form described in sections 3.1 and 3.2. The α_\pm and β_\pm parameters are varied in the two figures, respectively.

4. Odd p

In this section, we consider the case where the bulk anisotropy parameter assumes the values (1.3) with p odd, i.e., $\eta = \frac{i\pi}{2}, \frac{i\pi}{4}, \dots$. As for the even p case, for suitable values

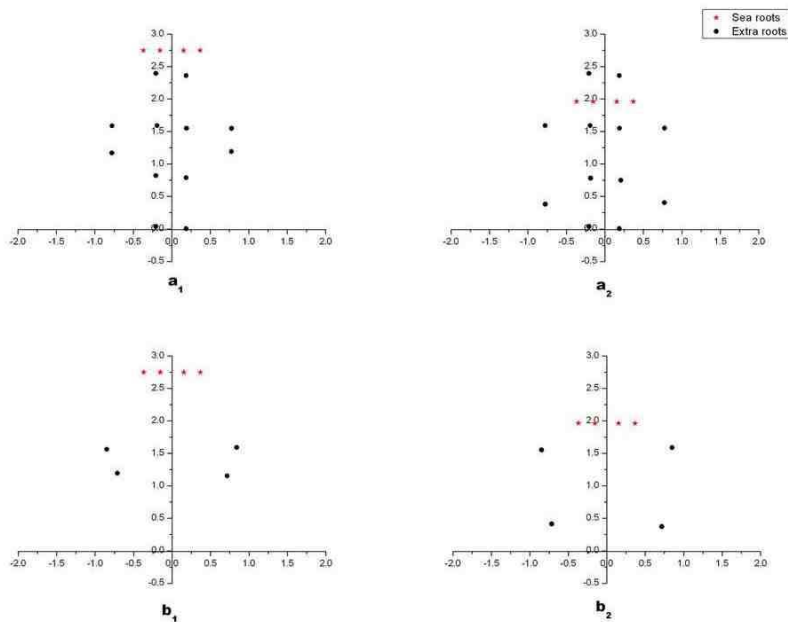


Figure 4: Ground-state Bethe roots for $p = 3$, $N = 4$, $\alpha_- = 1.554i$, $\alpha_+ = 0.948i$, $\beta_- = -0.214$, $\beta_+ = 0.186$, $\theta_- = 0.6i$, $\theta_+ = 0.7i$.

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 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”.

4.1 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

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

$$j = 1, \dots, \frac{p+1}{2}, \tag{4.1}$$

where \tilde{v}_k are real and positive. In figure 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 .

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

We now describe the extra Bethe roots for odd p . In figure 4, the extra roots are indicated

with black circles. We start with the $p - 1$ extra roots of the $b_j(u)$ functions:

$$\begin{aligned} w_k^{\pm(b_j)} &= \pm \tilde{w}_k + (p - k)\eta, \quad k = 1, \dots, p - 2, \\ w_{p-1}^{\pm(b_j)} &= \pm \tilde{w}_{p-1} + \left(\frac{p + 2 - 2j}{2} \right) \eta, \quad j = 1, \dots, \frac{p + 1}{2}. \end{aligned} \quad (4.2)$$

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

$$\tilde{w}_k = \tilde{w}_{p-k-1}, \quad k = 1, \dots, \frac{p-3}{2}, \quad (4.3)$$

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

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

$$\begin{aligned} w_k^{\pm(a_j,1)} &= w_k^{\pm(b_j)} = \pm \tilde{w}_k + (p - k)\eta, \quad k = 1, \dots, p - 2, \\ w_{p-1}^{\pm(a_j,1)} &= w_{p-1}^{\pm(b_j)} = \pm \tilde{w}_{p-1} + \left(\frac{p + 2 - 2j}{2} \right) \eta, \\ w_k^{\pm(a_j,2)} &= \pm \tilde{w}_0 + (p + 1 - k)\eta, \quad k = 1, \dots, p + 1, \quad j = 1, \dots, \frac{p + 1}{2}. \end{aligned} \quad (4.4)$$

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.

4.3 Boundary energy

As in the case of even p , we use the energy expression (2.19) and the string hypothesis to obtain (for $p \geq 3$)

$$\begin{aligned} E &= \frac{1}{2} \sinh \eta \left\{ \sum_{k=1}^{\frac{N}{2}} \left[\coth(v_k^{+(b_j)} + (j - 1)\eta) + \coth(v_k^{-(b_j)} + (j - 1)\eta) \right. \right. \\ &\quad \left. \left. - \coth(v_k^{+(b_{j-1})} + (j - 1)\eta) - \coth(v_k^{-(b_{j-1})} + (j - 1)\eta) \right] \right. \\ &\quad \left. + \sum_{k=1}^{p-1} \left[\coth(w_k^{+(b_j)} + (j - 1)\eta) + \coth(w_k^{-(b_j)} + (j - 1)\eta) \right. \right. \\ &\quad \left. \left. - \coth(w_k^{+(b_{j-1})} + (j - 1)\eta) - \coth(w_k^{-(b_{j-1})} + (j - 1)\eta) \right] \right\} + E_0, \\ j &= 2, \dots, \frac{p + 1}{2}. \end{aligned} \quad (4.5)$$

Recalling (4.1) and (4.2), this expression for the energy reduces, independently of the value of j , to

$$E = \sinh^2 \eta \sum_{k=1}^{\frac{N}{2}} \frac{1}{\sinh(\tilde{v}_k - \frac{\eta}{2}) \sinh(\tilde{v}_k + \frac{\eta}{2})} - \frac{2 \sinh^2 \eta}{\cosh \eta + \cosh(2\tilde{w}_{p-1})} + E_0, \quad (4.6)$$

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,

$$A_1 = A_2 = \dots = A_{\frac{p+1}{2}}, \quad B_1 = B_2 = \dots = B_{\frac{p+1}{2}}. \quad (4.7)$$

Choosing $u_l^{(b_j)}$ in (2.9) to be a sea root $v_l^{+(b_j)}$ for any $j \in \{2, \dots, \frac{p+1}{2}\}$, we obtain

$$\begin{aligned} & \left(\frac{\sinh(\tilde{v}_l + \frac{\eta}{2})}{\sinh(\tilde{v}_l - \frac{\eta}{2})} \right)^{2N} \frac{\sinh(2\tilde{v}_l + \eta) \sinh(\tilde{v}_l - \frac{\eta}{2} + \alpha_-) \cosh(\tilde{v}_l - \frac{\eta}{2} + \beta_-)}{\sinh(2\tilde{v}_l - \eta) \sinh(\tilde{v}_l + \frac{\eta}{2} - \alpha_-) \cosh(\tilde{v}_l + \frac{\eta}{2} - \beta_-)} \\ & \times \frac{\sinh(\tilde{v}_l - \frac{\eta}{2} + \alpha_+) \cosh(\tilde{v}_l - \frac{\eta}{2} + \beta_+)}{\sinh(\tilde{v}_l + \frac{\eta}{2} - \alpha_+) \cosh(\tilde{v}_l + \frac{\eta}{2} - \beta_+)} = - \frac{\sinh(\tilde{v}_l - \tilde{w}_{p-1} - \frac{p-1}{2}\eta) \sinh(\tilde{v}_l + \tilde{w}_{p-1} - \frac{p-1}{2}\eta)}{\sinh(\tilde{v}_l - \tilde{w}_{p-1} + \frac{p-1}{2}\eta) \sinh(\tilde{v}_l + \tilde{w}_{p-1} + \frac{p-1}{2}\eta)} \\ & \times \prod_{k=1}^{\frac{N}{2}} \frac{\sinh(\tilde{v}_l - \tilde{v}_k + \eta) \sinh(\tilde{v}_l + \tilde{v}_k + \eta)}{\sinh(\tilde{v}_l - \tilde{v}_k - \eta) \sinh(\tilde{v}_l + \tilde{v}_k - \eta)}, \quad l = 1, \dots, \frac{N}{2}, \quad \tilde{v}_k, \tilde{w}_{p-1} > 0. \end{aligned} \quad (4.8)$$

In a compact form, this result can be written as

$$\begin{aligned} e_1(\lambda_l)^{2N+1} g_1(\lambda_l) \frac{e_{2a_- - 1}(\lambda_l) e_{2a_+ - 1}(\lambda_l)}{g_{1+2ib_-}(\lambda_l) g_{1+2ib_+}(\lambda_l)} &= - [e_{p-1}(\lambda_l - \bar{\lambda}) e_{p-1}(\lambda_l + \bar{\lambda})]^{-1} \\ & \times \prod_{k=1}^{\frac{N}{2}} e_2(\lambda_l - \lambda_k) e_2(\lambda_l + \lambda_k), \quad l = 1, \dots, \frac{N}{2}, \end{aligned} \quad (4.9)$$

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

$$\begin{aligned} \mathfrak{h}(\lambda) &= \frac{1}{2\pi} \left\{ (2N+1)q_1(\lambda) + r_1(\lambda) + q_{2a_- - 1}(\lambda) - r_{1+2ib_-}(\lambda) + q_{2a_+ - 1}(\lambda) - r_{1+2ib_+}(\lambda) \right. \\ & \left. + q_{p-1}(\lambda - \bar{\lambda}) + q_{p-1}(\lambda + \bar{\lambda}) - \sum_{k=1}^{\frac{N}{2}} [q_2(\lambda - \lambda_k) + q_2(\lambda + \lambda_k)] \right\}. \end{aligned} \quad (4.10)$$

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

$$\begin{aligned} \rho(\lambda) &= 2a_1(\lambda) - \int_{-\infty}^{\infty} d\lambda' a_2(\lambda - \lambda') \rho(\lambda') + \frac{1}{N} \left[a_1(\lambda) + b_1(\lambda) + a_2(\lambda) \right. \\ & \left. + a_{2a_- - 1}(\lambda) - b_{1+2ib_-}(\lambda) + a_{2a_+ - 1}(\lambda) - b_{1+2ib_+}(\lambda) + a_{p-1}(\lambda - \bar{\lambda}) + a_{p-1}(\lambda + \bar{\lambda}) \right], \end{aligned} \quad (4.11)$$

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

$$\rho(\lambda) = 2s(\lambda) + \frac{1}{N}R(\lambda), \quad (4.12)$$

where now

$$\begin{aligned} \hat{R}(\omega) = \frac{1}{(1 + \hat{a}_2(\omega))} & \left\{ \hat{a}_1(\omega) + \hat{b}_1(\omega) + \hat{a}_2(\omega) - \hat{b}_{1+2ib_-}(\omega) - \hat{b}_{1+2ib_+}(\omega) \right. \\ & \left. + \hat{a}_{2a_- - 1}(\omega) + \hat{a}_{2a_+ - 1}(\omega) + 2 \cos(\bar{\lambda}\omega) \hat{a}_{p-1}(\omega) \right\}. \end{aligned} \quad (4.13)$$

The energy expression (4.6) yields, as $N \rightarrow \infty$,

$$\begin{aligned} E &= -\frac{2\pi \sin \mu}{\mu} \left\{ \sum_{k=1}^{\frac{N}{2}} a_1(\lambda_k) + b_1(\bar{\lambda}) \right\} + E_0 \\ &= -\frac{\pi \sin \mu}{\mu} \left\{ \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} a_1(\lambda_k) - a_1(0) + 2b_1(\bar{\lambda}) \right\} + E_0 \\ &= -\frac{\pi \sin \mu}{\mu} \left\{ N \int_{-\infty}^{\infty} d\lambda a_1(\lambda) \rho(\lambda) - a_1(0) + 2b_1(\bar{\lambda}) \right\} + \frac{1}{2}(N-1) \cos \mu \\ &\quad + \frac{1}{2} \sin \mu (\cot \mu a_- + i \tanh \mu b_- + \cot \mu a_+ + i \tanh \mu b_+). \end{aligned} \quad (4.14)$$

Substituting (4.12) for the root density, we again obtain

$$E = E_{\text{bulk}} + E_{\text{boundary}}, \quad (4.15)$$

where the bulk (order N) energy is again given by (3.25). The boundary energy is now given by

$$\begin{aligned} E_{\text{boundary}} &= -\frac{\pi \sin \mu}{\mu} I - \frac{1}{2} \cos \mu + \frac{1}{2} \sin \mu (\cot \mu a_- + i \tanh \mu b_- + \cot \mu a_+ + i \tanh \mu b_+) \\ &\quad - \frac{2\pi \sin \mu}{\mu} b_1(\bar{\lambda}), \end{aligned} \quad (4.16)$$

where I is now the integral

$$\begin{aligned} I &= \int_{-\infty}^{\infty} d\lambda a_1(\lambda) [R(\lambda) - \delta(\lambda)] = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \hat{a}_1(\omega) [\hat{R}(\omega) - 1] \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \hat{s}(\omega) \left\{ \hat{a}_1(\omega) + \hat{b}_1(\omega) - 1 \right. \\ &\quad \left. - \hat{b}_{1+2ib_-}(\omega) - \hat{b}_{1+2ib_+}(\omega) + \hat{a}_{2a_- - 1}(\omega) + \hat{a}_{2a_+ - 1}(\omega) + 2 \cos(\bar{\lambda}\omega) \hat{a}_{p-1}(\omega) \right\}. \end{aligned} \quad (4.17)$$

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 (4.16) 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

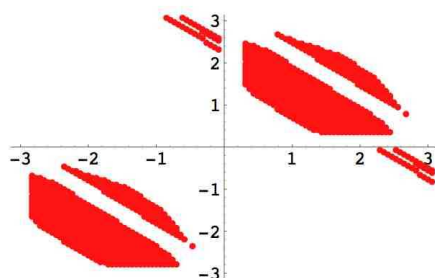


Figure 5: Shaded area denotes region of the $(\Im m \alpha_+, \Im m \alpha_-)$ plane for which the ground-state Bethe roots obey the string hypothesis for $p = 3$, $N = 2$, $\beta_- = -0.85$, $\beta_+ = 0.9$, $\theta_- = 0.6i$, $\theta_+ = 0.7i$.

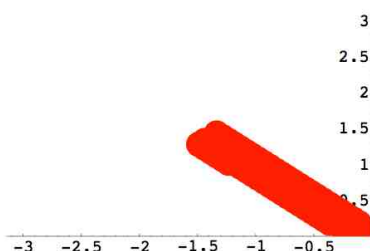


Figure 6: Shaded area denotes region of the (β_+, β_-) plane for which the ground-state Bethe roots obey the string hypothesis for $p = 3$, $N = 2$, $\alpha_- = 1.2i$, $\alpha_+ = 0.98i$, $\theta_- = 0.7i$, $\theta_+ = 0.6i$.

that the energy contribution from each boundary is again given by (3.28), thus coinciding with previous results in [21, 22].

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 and 6 denote the regions of parameter space for which the ground-state Bethe roots have the form described in sections 4.1 and 4.2. The α_{\pm} and β_{\pm} parameters are varied in the two figures, respectively.

5. Discussion

We have studied the ground state of the general integrable open XXZ spin-1/2 chain (1.1) in the thermodynamic limit, utilizing the solution we found recently in [19]. In contrast to the earlier solution [6–9], this solution does not assume any restrictions or constraints among the boundary parameters. However, the bulk parameter is restricted to values corresponding to roots of unity (1.3). 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 (3.28) was obtained previously [21] 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 [2], which is closely related to the open XXZ chain, the expression [24] for the boundary energy is valid for general values of the bulk and boundary parameters. In view of the spectral equivalence between systems with diagonal and nondiagonal boundary interactions noted in [11, 15, 16], it may be interesting to try to relate our boundary energy result with the corresponding result [20] for diagonal boundary interactions.

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., (2.19), (2.21)), and we find that the Bethe Ansatz equations (2.7), (2.9) 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.

Acknowledgments

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A. Expressions for $f_1(u)$ and μ_k

We list here explicit expressions for the function $f_1(u)$ and the coefficients μ_k appearing in the text. We remind the reader that we assume throughout that N is even.

For even values of p , the function $f_1(u)$ appearing in the Bethe Ansatz equations (2.6)–(2.9), (2.18) is given by

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

For odd values of p ,

$$f_1(u) = -2^{3-2p} \left(\begin{aligned} & \cosh((p+1)\alpha_-) \cosh((p+1)\beta_-) \cosh((p+1)\alpha_+) \cosh((p+1)\beta_+) \sinh^2((p+1)u) \\ & - \sinh((p+1)\alpha_-) \sinh((p+1)\beta_-) \sinh((p+1)\alpha_+) \sinh((p+1)\beta_+) \cosh^2((p+1)u) \\ & + \cosh((p+1)(\theta_- - \theta_+)) \sinh^2((p+1)u) \cosh^2((p+1)u) \end{aligned} \right). \quad (\text{A.2})$$

For both even and odd values of p , these functions have the properties

$$f_1(u + \eta) = f_1(u), \quad f_1(-u) = f_1(u). \quad (\text{A.3})$$

The coefficients μ_k appearing in the function $Y(u)$ (2.13) are given as follows for even (upper sign) and odd (lower sign) values of p .

$$\begin{aligned} \mu_0 &= 2^{-4p} \left\{ \begin{aligned} & -1 - \cosh^2((p+1)(\theta_- - \theta_+)) \\ & - \cosh(2(p+1)\alpha_-) \cosh(2(p+1)\alpha_+) \mp \cosh(2(p+1)\alpha_-) \cosh(2(p+1)\beta_-) \\ & \mp \cosh(2(p+1)\alpha_+) \cosh(2(p+1)\beta_-) \mp \cosh(2(p+1)\alpha_-) \cosh(2(p+1)\beta_+) \\ & \mp \cosh(2(p+1)\alpha_+) \cosh(2(p+1)\beta_+) - \cosh(2(p+1)\beta_-) \cosh(2(p+1)\beta_+) \\ & + \left[\cosh((p+1)(\alpha_- + \alpha_+)) \cosh((p+1)(\beta_- - \beta_+)) \right. \\ & \left. \pm \cosh((p+1)(\alpha_- - \alpha_+)) \cosh((p+1)(\beta_- + \beta_+)) \right]^2 \\ & \mp 2 \cosh((p+1)(\theta_- - \theta_+)) \left[\cosh((p+1)(\alpha_- - \alpha_+)) \cosh((p+1)(\beta_- - \beta_+)) \right. \\ & \left. \pm \cosh((p+1)(\alpha_- + \alpha_+)) \cosh((p+1)(\beta_- + \beta_+)) \right] \end{aligned} \right\}, \\ \mu_1 &= 2^{1-4p} \left\{ \begin{aligned} & \cosh((p+1)(\alpha_- \mp \alpha_+)) \left[\cosh((p+1)(\alpha_- \pm \alpha_+)) \right. \\ & \left. + \cosh((p+1)(\beta_- \pm \beta_+)) \cosh((p+1)(\theta_- - \theta_+)) \right] \\ & \mp \cosh((p+1)(\beta_- \mp \beta_+)) \left[\cosh((p+1)(\beta_- \pm \beta_+)) \right. \\ & \left. + \cosh((p+1)(\alpha_- \pm \alpha_+)) \cosh((p+1)(\theta_- - \theta_+)) \right] \end{aligned} \right\}, \\ \mu_2 &= 2^{-4p} \sinh^2((p+1)(\theta_- - \theta_+)). \end{aligned} \quad (\text{A.4})$$

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