

# Completeness of the Bethe Ansatz solution of the open XXZ chain with nondiagonal boundary terms

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## Abstract

A Bethe Ansatz solution of the open spin- $\frac{1}{2}$  XXZ quantum spin chain with non-diagonal boundary terms has recently been proposed. Using a numerical procedure developed by McCoy *et al.*, we find significant evidence that this solution can yield the complete set of eigenvalues for generic values of the bulk and boundary parameters satisfying one linear relation. Moreover, our results suggest that this solution is practical for investigating the ground state of this model in the thermodynamic limit.

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# 1 Introduction

The Bethe Ansatz solution of the open spin- $\frac{1}{2}$  XXZ quantum spin chain with diagonal boundary terms has long been known [1, 2]. However, the case of nondiagonal boundary terms [3] has resisted solution for many years (see, e.g., [4]). A Bethe Ansatz solution for the latter case has recently been proposed in [5, 6] (see also [7]). In terms of the parameters introduced there, the Hamiltonian is given by

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

where  $\sigma^x, \sigma^y, \sigma^z$  are the usual Pauli matrices,  $\eta$  is the bulk anisotropy parameter,  $\alpha_{\pm}, \beta_{\pm}, \theta_{\pm}$  are boundary parameters, and  $N$  is the number of spins. An unusual feature of this Bethe Ansatz solution is that the boundary parameters must satisfy the linear relation

$$\alpha_- + \beta_- + \alpha_+ + \beta_+ = \pm(\theta_- - \theta_+) + \eta k, \quad (1.2)$$

where  $k$  is an even integer if  $N$  is odd, and is an odd integer if  $N$  is even.<sup>1</sup> The energy eigenvalues are given by [6]

$$\begin{aligned} E = & \sinh^2 \eta \sum_{j=1}^M \frac{1}{\sinh u_j \sinh(u_j + \eta)} + \frac{1}{2} \sinh \eta (\coth \alpha_- + \tanh \beta_- + \coth \alpha_+ + \tanh \beta_+) \\ & + \frac{1}{2} (N - 1) \cosh \eta, \quad (1.3) \end{aligned}$$

where the Bethe roots  $\{u_j\}$  satisfy the Bethe Ansatz equations

$$\frac{h(u_j)}{h(-u_j - \eta)} = -\frac{Q(u_j + \eta)}{Q(u_j - \eta)}, \quad j = 1, \dots, M, \quad (1.4)$$

where  $h(u)$  is given by<sup>2</sup>

$$\begin{aligned} h(u) = & -\sinh^{2N}(u + \eta) \frac{\sinh(2u + 2\eta)}{\sinh(2u + \eta)} \\ & \times 4 \sinh(u + \alpha_-) \cosh(u + \beta_-) \sinh(u + \alpha_+) \cosh(u + \beta_+), \quad (1.5) \end{aligned}$$

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<sup>1</sup>An alternative solution was proposed in [8] which does not require any constraint among the boundary parameters. However, that solution holds only for  $\eta$  values corresponding to roots of unity, and the Bethe Ansatz equations are not of the conventional form.

<sup>2</sup>This expression for  $h(u)$  differs from (3.26) in [6] by the factors  $\kappa_- \kappa_+$  as the result of working here with a rescaled transfer matrix, as discussed further in Section 2.1.

and  $Q(u)$  is given by

$$Q(u) = \prod_{j=1}^M \sinh(u - u_j) \sinh(u + u_j + \eta), \quad (1.6)$$

which satisfies  $Q(u) = Q(-u - \eta)$ . The Bethe Ansatz equations assume a more symmetric form if expressed in terms of the shifted Bethe roots

$$\tilde{u}_j \equiv u_j + \frac{\eta}{2}. \quad (1.7)$$

Another unusual feature of this solution is that the number  $M$  of Bethe roots is fixed for given values of  $N$  and  $k$  (similar to the case of the XYZ chain), and is given by

$$M = \frac{1}{2}(N - 1 + k), \quad (1.8)$$

where  $k$  is the integer appearing in (1.2).

Several important issues were left unresolved in [6]. In particular, the Bethe Ansatz solution was obtained for the specific values of the anisotropy parameter  $\eta = i\pi/2, i\pi/4, \dots$  (for which  $q = e^\eta$  equals certain roots of unity). The solution was conjectured to hold for generic values of  $\eta$ , but little direct evidence was given. Also, because the value of the integer  $k$  in the constraint (1.2) is tied to the number of Bethe roots through (1.8), it is evident that the requirement of completeness should restrict the value of  $k$ . However, the problem of determining those restrictions remained unsolved.

The purpose of this article is to address these and related questions. From numerical studies of chains with sizes up to  $N = 7$ , we find significant evidence that the Bethe Ansatz solution indeed holds for generic values of  $\eta$ . In particular, for generic values of both bulk and boundary parameters, the Bethe Ansatz solution yields the *complete* set of  $2^N$  eigenvalues when  $k = N + 1$  (i.e.,  $M = N$ ). While it is gratifying to obtain all the eigenvalues, this result is also disappointing, as it is impractical to satisfy the constraint (1.2) with  $k = N + 1$  in the thermodynamic ( $N \rightarrow \infty$ ) limit. However, in practice one is interested primarily in the lowest-lying levels; and we find significant evidence that the Bethe Ansatz solution yields the *ground state* energy with just  $k = 1$  (i.e.,  $M = \frac{1}{2}N$ ) for  $N$  even, and with  $k = 0$  (i.e.,  $M = \frac{1}{2}(N - 1)$ ) for  $N$  odd. We also investigate the special case

$$\alpha_- = -\alpha_+, \quad \beta_- = -\beta_+, \quad \theta_+ = \theta_- = 0, \quad N = \text{odd} \quad (1.9)$$

considered in [5], and find evidence that the Bethe Ansatz solution gives the *complete* set of eigenvalues with  $k = 0$ .

The outline of this article is as follows. In Section 2, we consider the Bethe Ansatz solution for generic values of both bulk and boundary parameters. We describe an ingenious

procedure, which was pioneered by Barry McCoy and his collaborators, for addressing the problem of completeness; and we present the results we have obtained using this procedure. In Section 3 we consider the special case (1.9). We conclude with a summary of our main results in Section 4.

## 2 Generic case

We begin by addressing the following question: given a value of  $N$ , what value of  $k$  is needed to obtain from the Bethe Ansatz solution (1.2) - (1.8) the complete set of energy eigenvalues? To clarify the meaning of this question, let us make the elementary observation that the number of Bethe roots must satisfy  $M \geq 0$ ; hence, (1.8) implies that  $k$  must satisfy  $k \geq 1 - N$ . The minimum value  $k = 1 - N$  corresponds to zero Bethe roots, and therefore, to only **one** eigenvalue. (See Eq. (1.3).) Since a chain with  $N$  spins has  $2^N$  eigenvalues (which are distinct for generic values of parameters), this minimum value of  $k$  can give a complete set of eigenvalues only for  $N = 0$ .<sup>3</sup> We wish to determine, for higher values of  $N$ , the value(s) of  $k$  needed to obtain from the Bethe Ansatz solution the complete set of  $2^N$  eigenvalues.

Such questions of completeness are notoriously difficult to address, even numerically. Indeed, since there is no known systematic way of solving Bethe Ansatz equations, it is not possible to decide unequivocally when one has found all the solutions of those equations. Fortunately, there does exist a systematic method, exploited by McCoy and his collaborators (see, e.g. [9, 10]), of determining the Bethe roots corresponding to a given eigenvalue. Since, for small values of  $N$ , the eigenvalues can be computed by direct diagonalization, this method can be used to determine whether the Bethe Ansatz solution reproduces all the known eigenvalues. (Since in this approach one does not actually “solve” the Bethe Ansatz equations, the possibility remains open that those equations may admit additional solutions which do not correspond to actual eigenvalues. We shall return to this point later in Section 2.3.)

This method, to which we refer as ‘McCoy’s method’, actually makes use of the full transfer matrix of the model, rather than the Hamiltonian. Hence, we now briefly review its construction.

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<sup>3</sup>Although the Hamiltonian (1.1) makes sense only for  $N \geq 2$ , the transfer matrix (which is described below) is well-defined even for  $N = 0$ .

## 2.1 Transfer matrix

The transfer matrix for the open chain (1.1) is constructed according to Sklyanin's recipe [2] from the  $R$  matrix

$$R(u) = \begin{pmatrix} \sinh(u + \eta) & 0 & 0 & 0 \\ 0 & \sinh u & \sinh \eta & 0 \\ 0 & \sinh \eta & \sinh u & 0 \\ 0 & 0 & 0 & \sinh(u + \eta) \end{pmatrix} \quad (2.1)$$

and the  $2 \times 2$  nondiagonal matrices  $K^\mp(u)$  whose components are given by [3, 11]

$$\begin{aligned} K_{11}^-(u) &= 2(\sinh \alpha_- \cosh \beta_- \cosh u + \cosh \alpha_- \sinh \beta_- \sinh u) \\ K_{22}^-(u) &= 2(\sinh \alpha_- \cosh \beta_- \cosh u - \cosh \alpha_- \sinh \beta_- \sinh u) \\ K_{12}^-(u) &= e^{\theta_-} \sinh 2u, \quad K_{21}^-(u) = e^{-\theta_-} \sinh 2u, \end{aligned} \quad (2.2)$$

and

$$\begin{aligned} K_{11}^+(u) &= -2(\sinh \alpha_+ \cosh \beta_+ \cosh(u + \eta) - \cosh \alpha_+ \sinh \beta_+ \sinh(u + \eta)) \\ K_{22}^+(u) &= -2(\sinh \alpha_+ \cosh \beta_+ \cosh(u + \eta) + \cosh \alpha_+ \sinh \beta_+ \sinh(u + \eta)) \\ K_{12}^+(u) &= -e^{\theta_+} \sinh 2(u + \eta), \quad K_{21}^+(u) = -e^{-\theta_+} \sinh 2(u + \eta). \end{aligned} \quad (2.3)$$

The matrices  $K^\mp(u)$  are equal to those appearing in [6] divided by the factors  $\kappa_\mp$ , respectively. This leads to the rescaling of the transfer matrix already mentioned in Footnote 2.

The transfer matrix  $t(u)$  is given by [2]

$$t(u) = \text{tr}_0 K_0^+(u) T_0(u) K_0^-(u) \hat{T}_0(u), \quad (2.4)$$

where the monodromy matrices are given by

$$T_0(u) = R_{0N}(u) \cdots R_{01}(u), \quad \hat{T}_0(u) = R_{01}(u) \cdots R_{0N}(u), \quad (2.5)$$

and  $\text{tr}_0$  denotes trace over the ‘‘auxiliary space’’ 0. The transfer matrix has the important commutativity property

$$[t(u), t(v)] = 0, \quad (2.6)$$

and it ‘‘contains’’ the Hamiltonian (1.1),

$$\mathcal{H} = c_1 \frac{\partial}{\partial u} t(u) \Big|_{u=0} + c_2 \mathbb{I}, \quad (2.7)$$

where

$$\begin{aligned} c_1 &= \frac{1}{16 \sinh \alpha_- \cosh \beta_- \sinh \alpha_+ \cosh \beta_+ \sinh^{2N-1} \eta \cosh \eta}, \\ c_2 &= -\frac{\sinh^2 \eta + N \cosh^2 \eta}{2 \cosh \eta}, \end{aligned} \quad (2.8)$$

and  $\mathbb{I}$  is the identity matrix. According to the Bethe Ansatz solution [6], the eigenvalues  $\Lambda(u)$  of the transfer matrix are given by

$$\Lambda(u) = h(u) \frac{Q(u-\eta)}{Q(u)} + h(-u-\eta) \frac{Q(u+\eta)}{Q(u)}, \quad (2.9)$$

where  $h(u)$  and  $Q(u)$  are given by (1.5) and (1.6), respectively. The formula (1.3) for the energy eigenvalues follows directly from (2.7) - (2.9).

## 2.2 McCoy's method

To implement McCoy's method, it is more convenient to work with the spectral parameter  $x \equiv e^u$  and the anisotropy parameter  $q \equiv e^\eta$ . We denote by  $t(x)$  the transfer matrix expressed in terms of  $x$ , and similarly for other quantities.

McCoy's method consists of four steps: <sup>4</sup>

1. Fixing an arbitrary value  $x_0$  of the spectral parameter, compute numerically the eigenvectors  $|\Lambda\rangle$  of the transfer matrix  $t(x_0)$ . Due to the commutativity property of the transfer matrix, the eigenvectors do not depend on the spectral parameter.
2. Determine the eigenvalues  $\Lambda(x)$  by acting with  $t(x)$  on the eigenvectors  $|\Lambda\rangle$ . Due to the commutativity property of the transfer matrix, these eigenvalues are Laurent polynomials in  $x$ .
3. Set  $Q(x) = \sum_{k=0}^M b_k (x^{2k} + (xq)^{-2k})$  (see (1.6)), and determine the coefficients  $\{b_k\}$  from the relation (2.9), i.e.,  $\Lambda(x)Q(x) = h(x)Q(\frac{x}{q}) + h(\frac{1}{xq})Q(xq)$ .
4. Factor the polynomials  $Q(x)$ , whose zeros  $x_j$  are the sought-after Bethe roots.

Below we present the results that we have obtained using this method. We discuss separately the "massless" regime ( $\eta$  is purely imaginary) and the "massive" regime ( $\eta$  is purely real).

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<sup>4</sup>We are grateful to B. McCoy for explaining this procedure to us.

## 2.3 Massless regime

For the case that the bulk anisotropy parameter  $\eta$  is purely imaginary, the transfer matrix is generally not Hermitian. Hence, in principle, it may have fewer than  $2^N$  eigenvectors. Nevertheless, if the boundary parameters are suitably restricted, the transfer matrix can be shown to be a normal matrix, i.e.,

$$[t(u), t(u)^\dagger] = 0, \quad (2.10)$$

which implies that it is unitarily diagonalizable. Indeed, treating the spectral parameter  $u$  as real, it is easy to see that the  $R$  matrix (2.1) satisfies  $R(u)^\dagger = -R(-u)$ . Let us now restrict the boundary parameters so that

$$\alpha_\mp, \theta_\mp = \text{purely imaginary}, \quad \beta_\mp = \text{purely real}. \quad (2.11)$$

The  $K$  matrices (2.2), (2.3) then obey similar relations  $K^\mp(u)^\dagger = -K^\mp(-u)$ . It follows that the transfer matrix obeys the simple relation

$$t(u)^\dagger = t(-u). \quad (2.12)$$

Combining this result with the commutativity relation (2.6) immediately yields the desired result (2.10). Moreover, the conditions (2.11) for the boundary parameters imply that the Hamiltonian (1.1) is Hermitian.

In the numerical work which we present below, the values of the bulk and boundary parameters are chosen as follows:

$$\begin{aligned} \eta &= 0.3i, & \alpha_+ &= 0.75i, & \beta_+ &= -0.5, & \theta_+ &= 0.8i, \\ \alpha_- &= 0.25i + (k-1)(0.3i), & \beta_- &= 0.5, & \theta_- &= 0.1i. \end{aligned} \quad (2.13)$$

This set of values satisfies the constraint (1.2) for any value of  $k$ , as well as (2.11).

Table 1 shows, for values of  $N$  ranging from 0 to 4, all the  $2^N$  energy eigenvalues and the corresponding shifted Bethe roots. Our main observation is that, for each value of  $N$ , the corresponding value of  $k$  is equal to  $N + 1$ . (We obtained similar results for up to  $N = 7$ , but we do not present the data here.) For  $k > N + 1$ , the Bethe Ansatz also yields all  $2^N$  energy eigenvalues. But for  $1 - N \leq k < N + 1$ , the Bethe Ansatz does **not** yield all  $2^N$  energy eigenvalues.<sup>5</sup> In other words, the minimum value of  $k$  for which the Bethe Ansatz reproduces all the eigenvalues is  $k = N + 1$ . We have observed this numerically for the choice

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<sup>5</sup>For the “missing” eigenvalues (i.e., those eigenvalues of the transfer matrix which are not given by the Bethe Ansatz solution), step 3 of McCoy’s method fails: for such eigenvalues  $\Lambda(x)$ , there are no appropriate polynomials  $Q(x)$  which satisfy  $\Lambda(x)Q(x) = h(x)Q(\frac{x}{q}) + h(\frac{1}{xq})Q(xq)$ .

of parameters (2.13) with values of  $N$  up to 7, and we conjecture that it is true for generic values of the boundary parameters for all  $N$ .

We further conjecture that for  $k > N + 1$ , the Bethe Ansatz equations (6) admit extraneous solutions, which do not correspond to eigenvalues of the transfer matrix. We have verified this numerically for  $N = 0$  with  $k = 3$ . Indeed, with the choice of boundary parameters (2.13), we find for this case not only the Bethe root  $\tilde{u} = 0.690849 + 1.5708i$  which corresponds to the (single) transfer matrix eigenvalue, but also an additional solution of the Bethe Ansatz equation  $\tilde{u} = 1.4208i$  which does **not** correspond to this eigenvalue. As emphasized in the beginning of Section 2, it is difficult to hunt for solutions of Bethe Ansatz equations, especially for higher values of  $N$  and  $M$ .

Assuming that these two conjectures are correct, it follows that the Bethe Ansatz yields all  $2^N$  eigenvalues and no extraneous solutions for precisely  $k = N + 1$ . While it is gratifying to obtain all the eigenvalues, this result is also disappointing, since the constraint (1.2) then implies that the imaginary parts of the boundary parameters should grow linearly with  $N$ .

### 2.3.1 Ground state

Although a high value of  $k$  is required to obtain all the energy levels (namely,  $k = N + 1$ ), we find that the ground-state energy can be obtained with a much lower value of  $k$ . Indeed, using the parameter values (2.13), we performed a search for the minimum value of  $k$  (for a given value of  $N$ ) where the Bethe Ansatz reproduces the ground-state energy, up to  $N = 7$ . Our results are summarized in Table 2, which gives in addition to the value of  $k$  also the ground-state energy and the corresponding Bethe roots. Our main observation here is that  $k = 0$  for  $N$  odd, and  $k = 1$  for  $N$  even. We conjecture that this result is true for generic values of the boundary parameters for all  $N$ . If correct, then the Bethe Ansatz is practical for investigating the ground state in the thermodynamic limit.

We also observe from Table 2 that the shifted Bethe roots are real for the ground state, as is also the case for the closed XXZ chain with periodic boundary conditions. (For higher values of  $k$ , the shifted Bethe roots for the ground state are either real or have imaginary parts  $i\pi/2$ , as can be seen from Table 1.)

Finally, we remark that our numerical results suggest that the Bethe Ansatz correctly yields  $2^{N-1}$  eigenvalues for  $k = 0$  ( $N$  odd), and  $2^{N-1} + \frac{1}{2}\binom{N}{N/2}$  eigenvalues for  $k = 1$  ( $N$  even).<sup>6</sup>

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<sup>6</sup>In formulating the latter conjecture, which we have checked up to  $N = 8$ , a useful reference was [12].

## 2.4 Massive regime

For the case that  $\eta$  is purely real, we choose  $\theta_{\mp} = 0$  and the remaining boundary parameters to be real, thereby making the transfer matrix manifestly Hermitian. In particular, for the numerical work presented below, we take the values

$$\begin{aligned}\eta &= 0.3, & \alpha_+ &= 0.75, & \beta_+ &= -1.2, & \theta_+ &= 0, \\ \alpha_- &= 0.25 + (k-1)(0.3), & \beta_- &= 0.5, & \theta_- &= 0,\end{aligned}\tag{2.14}$$

which satisfy the constraint (1.2) for any value of  $k$ .

Our results for the massive regime are very similar to those for the massless regime. Indeed, consider Table 3, which shows all the  $2^N$  energy eigenvalues and the corresponding Bethe roots for values of  $N$  ranging from 0 to 4. As in the massless case, the minimum value of  $k$  for which the Bethe Ansatz reproduces all the eigenvalues is  $k = N + 1$ . (We obtained similar results for  $N = 5$ . For larger values of  $N$ , roundoff errors become significant.) Moreover, as shown in Table 4, the Bethe Ansatz reproduces the ground state energy for  $k = 0$  for  $N$  odd, and  $k = 1$  for  $N$  even. The corresponding shifted Bethe roots are purely imaginary.

## 3 Special case

We now turn to the special case (1.9), which was first considered in [5]. In this case, the boundary terms of the Hamiltonian (1.1) reduce to

$$\frac{1}{2} \sinh \eta [\coth \alpha_- \tanh \beta_- (\sigma_1^z - \sigma_N^z) + \operatorname{csch} \alpha_- \operatorname{sech} \beta_- (\sigma_1^x - \sigma_N^x)].\tag{3.1}$$

We first argue that for this case all the energy eigenvalues are 2-fold degenerate. Indeed, it is easy to see that the Hamiltonian commutes with the operator  $U$  defined by <sup>7</sup>

$$U = C P,\tag{3.2}$$

where  $C$  is the ‘‘charge conjugation’’ operator

$$C = \prod_{n=1}^N \sigma_n^y,\tag{3.3}$$

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<sup>7</sup>A similar symmetry operator was invoked in [13] to argue that an open chain with *diagonal* boundary terms has a two-fold degenerate spectrum for  $N$  odd. There the argument is simpler, since in that case the Hamiltonian also commutes with  $S^z$ , while  $U$  and  $S^z$  anticommute.

which satisfies  $C^\dagger = C$  and  $C^2 = 1$ ; and  $P$  is the ‘‘parity’’ operator [14], which satisfies

$$P \sigma_n^j P = \sigma_{N+1-n}^j, \quad (3.4)$$

as well as  $P^\dagger = P$  and  $P^2 = 1$ . It follows that also  $U$  is Hermitian and squares to 1. Hence,  $U$  has eigenvalues  $\pm 1$ . For  $N$  odd,  $U$  has an equal number of  $+1$  and  $-1$  eigenvalues.<sup>8</sup> It follows that all energy eigenvalues are 2-fold degenerate. In fact, since  $U$  commutes with the full transfer matrix  $t(u)$ , all the eigenvalues  $\Lambda(u)$  are 2-fold degenerate.

Since for this case there are generally only  $2^{N-1}$  distinct eigenvalues, one expects that all of these eigenvalues can be reproduced by the Bethe Ansatz with a value of  $k < N + 1$ . Indeed, as shown in Table 5, we find significant evidence which supports the conjecture that the complete set of  $2^{N-1}$  eigenvalues is obtained for  $k = 0$  (i.e.,  $M = \frac{1}{2}(N - 1)$ ). (We obtained similar results for  $N = 7$ .)

## 4 Conclusion

Within the range of parameters which we have explored (as detailed in Sections 2.3 and 2.4), we have found significant numerical evidence for the following conjectures regarding the Bethe Ansatz solution (1.2) - (1.8) of the model (1.1):

- For generic values of the bulk and boundary parameters satisfying (1.2), the solution yields the complete set of  $2^N$  eigenvalues for  $k = N + 1$  (i.e.,  $M = N$ ).
- The solution yields the ground state energy for  $k = 1$  (i.e.,  $M = \frac{1}{2}N$ ) when  $N$  is even, and for  $k = 0$  (i.e.,  $M = \frac{1}{2}(N - 1)$ ) when  $N$  is odd. In the massless regime, the shifted Bethe roots corresponding to these states are real.
- In the special case (1.9) where the spectrum is 2-fold degenerate, the Bethe Ansatz solution yields the complete set of  $2^{N-1}$  eigenvalues for  $k = 0$  (i.e.,  $M = \frac{1}{2}(N - 1)$ ).

These results suggest that the Bethe Ansatz solution is both valid and practical for investigating the ground state (and presumably, also low-lying excited states) of the model

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<sup>8</sup>To prove this, it suffices to show that the trace of  $U$  is zero. For  $N$  odd, the parity operator leaves the ‘‘middle’’ spin at site  $\frac{1}{2}(N + 1)$  invariant. Hence,

$$\text{tr } U = \text{tr}_{12\dots N} U = \text{tr}_{\frac{1}{2}(N+1)} \left( \sigma_{\frac{1}{2}(N+1)}^y \right) \text{tr}' \left( P \prod_{n \neq \frac{1}{2}(N+1)} \sigma_n^y \right) = 0,$$

since the Pauli matrix  $\sigma^y$  is traceless. (Here  $\text{tr}'$  denotes trace over all spaces  $n \neq \frac{1}{2}(N + 1)$ .)

(1.1) in the thermodynamic limit. In particular, these results provide justification for the computations in [15] of the thermodynamic limit for the special case (1.9), and clear the way for analogous computations in the general case. We stress, however, that this model has many parameters, other ranges of which remain to be explored.

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### Note added:

There is a counterpart of the special case (1.9) for even values of  $N$ , namely,

$$\alpha_- = -\alpha_+ + \eta, \quad \beta_- = -\beta_+, \quad \theta_+ = \theta_- = 0, \quad N = \text{even},$$

and hence  $k = 1$ . For this case the spectrum also has degeneracies. For even values of  $N$  up to  $N = 6$ , we find that the Bethe Ansatz solution with  $M = \frac{1}{2}N$  gives the complete set of  $2^{N-1} + \frac{1}{2}\binom{N}{N/2}$  distinct eigenvalues.

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## ADDENDUM to “Completeness of the Bethe Ansatz solution of the open XXZ chain with nondiagonal boundary terms”

In [1] (to which we refer hereafter by I), we find significant numerical evidence that for the open XXZ quantum spin chain Hamiltonian (I1.1) with bulk and boundary parameters satisfying the constraint (I1.2)

$$\alpha_- + \beta_- + \alpha_+ + \beta_+ = \pm(\theta_- - \theta_+) + \eta k, \quad (1)$$

the Bethe Ansatz solution (I1.3) - (I1.8), (I2.9) gives the complete set of  $2^N$  eigenvalues for  $k = N + 1$ ; and this solution gives only some (but not all) of the eigenvalues for  $1 - N \leq k < N + 1$ . Here we conjecture that a simple generalization of this Bethe Ansatz solution gives the *complete* set of eigenvalues for *all* values of  $k$  in the interval  $-(N + 1) \leq k \leq N + 1$ .

Indeed, consider the following two expressions, distinguished by  $\pm$ , for the eigenvalues of the transfer matrix (I2.4):

$$\Lambda_{\pm}(u) = h_{\pm}(u) \frac{Q_{\pm}(u - \eta)}{Q_{\pm}(u)} + h_{\pm}(-u - \eta) \frac{Q_{\pm}(u + \eta)}{Q_{\pm}(u)}, \quad (2)$$

where  $h_{\pm}(u)$  are given by

$$\begin{aligned} h_{\pm}(u) &= -\sinh^{2N}(u + \eta) \frac{\sinh(2u + 2\eta)}{\sinh(2u + \eta)} \\ &\times 4 \sinh(u \pm \alpha_-) \cosh(u \pm \beta_-) \sinh(u \pm \alpha_+) \cosh(u \pm \beta_+); \end{aligned} \quad (3)$$

and  $Q_{\pm}(u)$  are given by

$$Q_{\pm}(u) = \prod_{j=1}^{M_{\pm}} \sinh(u - u_j^{\pm}) \sinh(u + u_j^{\pm} + \eta), \quad (4)$$

where

$$M_{\pm} = \frac{1}{2}(N - 1 \pm k). \quad (5)$$

The corresponding Bethe Ansatz equations are

$$\frac{h_{\pm}(u_j^{\pm})}{h_{\pm}(-u_j^{\pm} - \eta)} = -\frac{Q_{\pm}(u_j^{\pm} + \eta)}{Q_{\pm}(u_j^{\pm} - \eta)}, \quad j = 1, \dots, M_{\pm}. \quad (6)$$

The Bethe Ansatz solution considered earlier [2,1] corresponds to the above expressions with the plus (+) sign.

We conjecture that for a given set of bulk and boundary parameters satisfying (1) with  $|k| \leq N + 1$  and  $k$  odd (even) for  $N$  even (odd), the eigenvalues  $\Lambda_+(u)$  and  $\Lambda_-(u)$  together

give the complete set of eigenvalues of the transfer matrix. That is, for  $k = N + 1$ , all the eigenvalues are given by  $\Lambda_+(u)$  (as found in I); for  $k = -(N + 1)$ , all the eigenvalues are given by  $\Lambda_-(u)$ ; and for  $-(N + 1) < k < N + 1$ , both  $\Lambda_+(u)$  and  $\Lambda_-(u)$  are needed to obtain the complete set of eigenvalues.

This conjecture is supported by significant numerical evidence, obtained (as in I) using ‘McCoy’s method’. For instance, for  $N = 6$  and  $k = 1$ , we find that 42 eigenvalues are given by  $\Lambda_+(u)$  and 22 eigenvalues are given by  $\Lambda_-(u)$ ; together, they give the complete set of  $2^6 = 64$  eigenvalues.

## References

- [1] R.I. Nepomechie and F. Ravanini, “Completeness of the Bethe Ansatz solution of the open XXZ chain with nondiagonal boundary terms,” [hep-th/0307095](#)
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$N$	$k$	$M$	$E$	shifted Bethe roots $\tilde{u}_j$
0	1	0	0.259617	–
1	2	1	-0.455662	0.278824
			0.455662	$0.702627 + u_0$
2	3	2	-1.48624	$0.124133, 0.691313 + u_0$
			0.13202	$0.334031 \pm 0.186753i$
			0.483745	$0.467053, 0.678121 + u_0$
			0.870471	$0.55974 + u_0, 0.974697 + u_0$
3	4	3	-2.20345	$0.0866988, 0.373369, 0.655889 + u_0$
			-1.75971	$0.0794522, 0.542856 + u_0, 0.939102 + u_0$
			-0.0127446	$0.240758 \pm 0.139792i, 0.659713 + u_0$
			-0.00644228	$0.21088, 0.541397 + u_0, 0.935445 + u_0$
			0.671117	$0.39724, 0.362185 \pm 0.341578i$
			0.878343	$0.638761 + u_0, 0.511044 \pm 0.205038i$
			1.09747	$0.615979, 0.530429 + u_0, 0.906019 + u_0$
			1.33542	$0.468162 + u_0, 0.719202 + u_0, 1.16451 + u_0$
4	5	4	-3.20655	$0.0656969, 0.173673, 0.505631 + u_0, 0.869254 + u_0$
			-2.15365	$0.0641635, 0.601829 + u_0, 0.390452 \pm 0.193885i$
			-1.895	$0.0609306, 0.526013, 0.497497 + u_0, 0.847927 + u_0$
			-1.6139	$0.0587044, 0.432076 + u_0, 0.672212 + u_0, 1.10249 + u_0$
			-0.66516	$0.163048, 0.365317 \pm 0.193132i, 0.602513 + u_0$
			-0.549331	$0.145871, 0.515342, 0.497186 + u_0, 0.847232 + u_0$
			-0.345969	$0.136943, 0.431537 + u_0, 0.671367 + u_0, 1.101 + u_0$
			0.259969	$0.506611 + u_0, 0.87182 + u_0, 0.160443 \pm 0.150348i$
			0.842045	$0.287219, 0.297174 \pm 0.310653i, 0.609213 + u_0$
			0.891361	$0.497959 + u_0, 0.849881 + u_0, 0.370167 \pm 0.118987i$
			0.948984	$0.285065, 0.429407 + u_0, 0.668011 + u_0, 1.09495 + u_0$
			1.1934	$0.429338 \pm 0.160247i, 0.373211 \pm 0.475013i$
			1.33834	$0.56912, 0.582163 + u_0, 0.533392 \pm 0.368923i$
			1.48584	$0.48142 + u_0, 0.807965 + u_0, 0.649061 \pm 0.215203i$
			1.64707	$0.733488, 0.41686 + u_0, 0.647858 + u_0, 1.05404 + u_0$
			1.82255	$0.367461 + u_0, 0.570419 + u_0, 0.839668 + u_0, 1.29177 + u_0$

Table 1: Complete set of  $2^N$  energy levels and Bethe roots in the massless regime, using parameter values (2.13). We use the shorthand notation  $u_0 = i\pi/2$ . Without loss of generality, we restrict the shifted Bethe roots so that  $\Re e \tilde{u}_j > 0$  and  $-\frac{\pi}{2} < \Im m \tilde{u}_j \leq \frac{\pi}{2}$ .

$N$	$k$	$M$	ground-state energy $E$	shifted Bethe roots $\tilde{u}_j$
1	0	0	-2.79413	–
2	1	1	-1.57715	0.0944455
3	0	1	-4.58216	0.0973252
4	1	2	-3.3477	0.0559452, 0.139137
5	0	2	-6.35177	0.0572972, 0.14122
6	1	3	-5.10816	0.0402978, 0.0893334, 0.168789
7	0	3	-8.11181	0.0410605, 0.0906602, 0.170368

Table 2: Ground-state energy and Bethe roots in the massless regime, using parameter values (2.13).

$N$	$k$	$M$	$E$	shifted Bethe roots $\tilde{u}_j$
0	1	0	0.28216	–
1	2	1	-0.478182	0.274302 <i>i</i>
			0.478182	1.82287 + $u_0$
2	3	2	-1.52836	0.123806 <i>i</i> , 1.83483 + $u_0$
			0.128052	0.184296 ± 0.327865 <i>i</i>
			0.496614	0.460762 <i>i</i> , 1.84961 + $u_0$
			0.903692	1.44453 + $u_0$ , 2.2506 + $u_0$
3	4	3	-2.2733	0.0866767 <i>i</i> , 0.369644 <i>i</i> , 1.87489 + $u_0$
			-1.80933	0.0794024 <i>i</i> , 1.45356 + $u_0$ , 2.27091 + $u_0$
			-0.00928535	0.140292 ± 0.238892 <i>i</i> , 1.86994 + $u_0$
			-0.00463236	0.210583 <i>i</i> , 1.45452 + $u_0$ , 2.27283 + $u_0$
			0.684253	0.387332 <i>i</i> , 0.337297 ± 0.355183 <i>i</i>
			0.903368	0.202474 ± 0.507083 <i>i</i> , 1.89723 + $u_0$
			1.12743	0.608104 <i>i</i> , 1.46245 + $u_0$ , 2.28776 + $u_0$
			1.38149	1.36248 + $u_0$ , 1.78447 + $u_0$ , 2.59988 + $u_0$
4	5	4	-3.30164	0.0657087 <i>i</i> , 0.173726 <i>i</i> , 1.47329 + $u_0$ , 2.31403 + $u_0$
			-2.21969	0.0641814 <i>i</i> , 0.192461 ± 0.388014 <i>i</i> , 1.94346 + $u_0$
			-1.95389	0.0609669 <i>i</i> , 0.524409 <i>i</i> , 1.47997 + $u_0$ , 2.32536 + $u_0$
			-1.66252	0.0587306 <i>i</i> , 1.36591 + $u_0$ , 1.79991 + $u_0$ , 2.62653 + $u_0$
			-0.68481	0.191746 ± 0.362798 <i>i</i> , 0.163232 <i>i</i> , 1.94239 + $u_0$
			-0.56579	0.146007 <i>i</i> , 0.513987 <i>i</i> , 1.4802 + $u_0$ , 2.32576 + $u_0$
			-0.355209	0.137034 <i>i</i> , 1.36599 + $u_0$ , 1.80022 + $u_0$ , 2.62701 + $u_0$
			0.270674	0.150351 ± 0.160618 <i>i</i> , 1.47252 + $u_0$ , 2.31269 + $u_0$
			0.87254	0.310225 ± 0.295283 <i>i</i> , 0.285824 <i>i</i> , 1.93176 + $u_0$
			0.920906	0.119052 ± 0.37073 <i>i</i> , 1.47931 + $u_0$ , 2.32448 + $u_0$
			0.978875	0.285415 <i>i</i> , 1.36633 + $u_0$ , 1.80148 + $u_0$ , 2.62891 + $u_0$
			1.22216	0.158173 ± 0.41471 <i>i</i> , 0.46895 ± 0.364585 <i>i</i>
			1.38081	0.366909 ± 0.5330611 <i>i</i> , 0.565907 <i>i</i> , 1.97405 + $u_0$
			1.52904	0.212615 ± 0.654327 <i>i</i> , 1.49436 + $u_0$ , 2.34875 + $u_0$
			1.68784	0.724014 <i>i</i> , 1.36869 + $u_0$ , 1.80952 + $u_0$ , 2.64055 + $u_0$
			1.8807	1.35068 + $u_0$ , 1.66925 + $u_0$ , 2.10024 + $u_0$ , 2.91917 + $u_0$

Table 3: Complete set of  $2^N$  energy levels and Bethe roots in the massive regime, using parameter values (2.14). We use the shorthand notation  $u_0 = i\pi/2$ . Without loss of generality, we restrict the shifted Bethe roots so that  $\Re \tilde{u}_j > 0$  and  $-\frac{\pi}{2} < \Im \tilde{u}_j \leq \frac{\pi}{2}$ ; or  $\Re \tilde{u}_j = 0$  and  $0 < \Im \tilde{u}_j \leq \frac{\pi}{2}$ .

$N$	$k$	$M$	ground-state energy $E$	shifted Bethe roots $\tilde{u}_j$
1	0	0	-2.86459	–
2	1	1	-1.61648	$0.0941058i$
3	0	1	-4.71323	$0.0969713i$
4	1	2	-3.4432	$0.0558492i, 0.138676i$
5	0	2	-6.53887	$0.0571973i, 0.140752i$

Table 4: Ground-state energy and Bethe roots in the massive regime, using parameter values (2.14).

$N$	$k$	$M$	$E$	shifted Bethe roots $\tilde{u}_j$
1	0	0	0	–
3	0	1	-2.06361	$0.0811287$
			-0.202938	$0.228372$
			0.983167	$1.1779 + u_0$
5	0	2	1.28338	$0.567083i$
			-3.93243	$0.0518373, 0.121304$
			-2.55868	$0.0501521, 0.259987$
			-1.61887	$0.0470911, 1.18204 + u_0$
			-1.53627	$0.114268, 0.255101$
			-1.3471	$0.0452599, 0.570638i$
			-0.687493	$0.10434, 1.18027 + u_0$
			-0.474743	$0.0991988, 0.56857i$
			0.268219	$0.119246 \pm 0.149991i$
			0.486895	$0.19328, 1.17489 + u_0$
0.642915	$0.17875, 0.564459i$			
0.954064	$0.278324 \pm 0.155511i$			
1.49874	$0.407709, 1.14897 + u_0$			
1.65895	$0.347419, 0.557976i$			
1.96938	$0.850516 + u_0, 1.62572 + u_0$			
2.28162	$0.551706i, 1.24328 + u_0$			
2.3948	$0.550319i, 0.950981i$			

Table 5: Complete set of  $2^{N-1}$  energy levels and Bethe roots for the special case (1.9), with  $\eta = 0.3i$ ,  $\alpha_- = -\alpha_+ = 0.4i$ ,  $\beta_- = -\beta_+ = 0.7$ ,  $\theta_+ = \theta_- = 0$ . We use the shorthand notation  $u_0 = i\pi/2$ . Without loss of generality, we restrict the shifted Bethe roots so that  $\Re \tilde{u}_j > 0$  and  $-\frac{\pi}{2} < \Im \tilde{u}_j \leq \frac{\pi}{2}$ ; or  $\Re \tilde{u}_j = 0$  and  $0 < \Im \tilde{u}_j \leq \frac{\pi}{2}$ .