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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 nondiagonal 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

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

where $\sigma^x, \sigma^y, \sigma^z$ are the usual Pauli matrices, η 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

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

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where k is an even integer if N is odd, and is an odd integer if N is even[3]. The energy eigenvalues are given by [6]

$$E = \sinh^2\eta \sum_{j=1}^{M} \frac{1}{\sinh u_j \sinh(u_j+\eta)} + \frac{1}{2}\sinh\eta(\coth\alpha_- + \tanh\beta_- + \coth\alpha_+ + \tanh\beta_+) + \frac{1}{2}(N-1)\cosh\eta \tag{1.3}$$

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

$$\frac{h(u_j)}{h(-u_j-\eta)} = -\frac{Q(u_j+\eta)}{Q(u_j-\eta)} \qquad j = 1, \ldots, M \tag{1.4}$$

where $h(u)$ is given by[4]

$$h(u) = -\sinh^{2N}(u+\eta)\frac{\sinh(2u+2\eta)}{\sinh(2u+\eta)} 4\sinh(u+\alpha_-)\cosh(u+\beta_-)\sinh(u+\alpha_+)\cosh(u+\beta_+) \tag{1.5}$$

and $Q(u)$ is given by

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

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

$$\tilde{u}_j \equiv u_j + \frac{\eta}{2}. \tag{1.7}$$

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

$$M = \tfrac{1}{2}(N-1+k) \tag{1.8}$$

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 $\eta = \mathrm{i}\pi/2, \mathrm{i}\pi/4, \ldots$ (for which $q = \mathrm{e}^{\eta}$ equals certain roots of unity). The solution was conjectured to hold for generic values of η, 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 paper 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 η. 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 ($N \to \infty$) limit. However, in practice one is interested primarily in the lowest

[3] An alternative solution was proposed in [8] which does not require any constraint among the boundary parameters. However, that solution holds only for η values corresponding to roots of unity, and the Bethe Ansatz equations are not of the conventional form.

[4] 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.

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

$$\alpha_- = -\alpha_+ \qquad \beta_- = -\beta_+ \qquad \theta_+ = \theta_- = 0 \qquad N = \text{odd} \tag{1.9}$$

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

The outline of this paper 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 $M \geqslant 0$; hence, (1.8) implies that k must satisfy $k \geqslant 1 - N$. The minimum value $k = 1 - N$ corresponds to zero Bethe roots, and therefore, to only *one* eigenvalue. (See equation (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 $N = 0$.[5] 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.

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

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

[5] Although the Hamiltonian (1.1) makes sense only for $N \geqslant 2$, the transfer matrix (which is described below) is well defined even for $N = 0$.

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

$$\begin{aligned} K^{-}_{11}(u) &= 2(\sinh\alpha_- \cosh\beta_- \cosh u + \cosh\alpha_- \sinh\beta_- \sinh u) \\ K^{-}_{22}(u) &= 2(\sinh\alpha_- \cosh\beta_- \cosh u - \cosh\alpha_- \sinh\beta_- \sinh u) \\ K^{-}_{12}(u) &= \mathrm{e}^{\theta_-} \sinh 2u \qquad K^{-}_{21}(u) = \mathrm{e}^{-\theta_-} \sinh 2u \end{aligned} \tag{2.2}$$

and

$$\begin{aligned} K^{+}_{11}(u) &= -2(\sinh\alpha_+ \cosh\beta_+ \cosh(u+\eta) - \cosh\alpha_+ \sinh\beta_+ \sinh(u+\eta)) \\ K^{+}_{22}(u) &= -2(\sinh\alpha_+ \cosh\beta_+ \cosh(u+\eta) + \cosh\alpha_+ \sinh\beta_+ \sinh(u+\eta)) \\ K^{+}_{12}(u) &= -\mathrm{e}^{\theta_+} \sinh 2(u+\eta) \qquad K^{+}_{21}(u) = -\mathrm{e}^{-\theta_+} \sinh 2(u+\eta). \end{aligned} \tag{2.3}$$

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 4.

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

$$t(u) = \mathrm{tr}_0 K^{+}_0(u) T_0(u) K^{-}_0(u) \hat{T}_0(u) \tag{2.4}$$

where the monodromy matrices are given by

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

and tr_0 denotes trace over the 'auxiliary space' 0. The transfer matrix has the important commutativity property

$$[t(u), t(v)] = 0 \tag{2.6}$$

and it 'contains' the Hamiltonian (1.1),

$$\mathcal{H} = c_1 \left. \frac{\partial}{\partial u} t(u) \right|_{u=0} + c_2 \mathbb{I} \tag{2.7}$$

where

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

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

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

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 $x \equiv \mathrm{e}^u$ and the anisotropy parameter $q \equiv \mathrm{e}^\eta$. 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[6]:

[6] We are grateful to B McCoy for explaining this procedure to us.

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. $\Lambda(x)Q(x) = h(x)Q\left(\frac{x}{q}\right) + h\left(\frac{1}{xq}\right)Q(xq)$.
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 (η is purely imaginary) and the 'massive' regime (η is purely real).

2.3. *Massless regime*

For the case that the bulk anisotropy parameter η 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.

$$[t(u), t(u)^\dagger] = 0 \tag{2.10}$$

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

$$\alpha_\mp, \theta_\mp = \text{purely imaginary} \qquad \beta_\mp = \text{purely real}. \tag{2.11}$$

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

$$t(u)^\dagger = t(-u). \tag{2.12}$$

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:

$$\begin{array}{llll} \eta = 0.3\mathrm{i} & \alpha_+ = 0.75\mathrm{i} & \beta_+ = -0.5 & \theta_+ = 0.8\mathrm{i} \\ \alpha_- = 0.25\mathrm{i} + (k-1)(0.3\mathrm{i}) & & \beta_- = 0.5 & \theta_- = 0.1\mathrm{i}. \end{array} \tag{2.13}$$

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 $1 - N \leqslant k < N+1$, the Bethe Ansatz does *not* yield all 2^N energy eigenvalues[7]. 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

[7] 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 $\Lambda(x)Q(x) = h(x)Q(\frac{x}{q}) + h(\frac{1}{xq})Q(xq)$.

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 $u_0 = \mathrm{i}\pi/2$. Without loss of generality, we restrict the shifted Bethe roots so that $\mathrm{Re}\,\tilde{u}_j > 0$ and $-\frac{\pi}{2} < \mathrm{Im}\,\tilde{u}_j \leqslant \frac{\pi}{2}$.

N	k	M	E	Shifted Bethe roots $\tilde{u}_j$
0	1	0	0.259 617	–
1	2	1	−0.455 662	0.278 824
			0.455 662	0.702 627 + u_0
2	3	2	−1.486 24	0.124 133, 0.691 313 + u_0
			0.132 02	0.334 031 ± 0.186 753i
			0.483 745	0.467 053, 0.678 121 + u_0
			0.870 471	0.559 74 + u_0, 0.974 697 + u_0
3	4	3	−2.203 45	0.086 698 8, 0.373 369,0.655 889 + u_0
			−1.759 71	0.079 452 2, 0.542 856 + u_0, 0.939102 + u_0
			−0.012 744 6	0.240 758 ± 0.139 792i, 0.659 713 + u_0
			−0.006 442 28	0.210 88, 0.541 397 + u_0, 0.935 445 + u_0
			0.671 117	0.397 24, 0.362 185 ± 0.341 578i
			0.878 343	0.638 761 + u_0, 0.511 044 ± 0.205 038i
			1.097 47	0.615 979, 0.530 429 + u_0, 0.906 019 + u_0
			1.335 42	0.468 162 + u_0, 0.719 202 + u_0, 1.164 51 + u_0
4	5	4	−3.206 55	0.065 696 9, 0.173 673, 0.505 631 + u_0, 0.869 254 + u_0
			−2.153 65	0.064 163 5, 0.601 829 + u_0, 0.390 452 ± 0.193 885i
			−1.895	0.060 930 6, 0.526 013, 0.497 497 + u_0, 0.847 927 + u_0
			−1.613 9	0.058 704 4, 0.432 076 + u_0, 0.672 212 + u_0, 1.102 49 + u_0
			−0.665 16	0.163 048, 0.365 317 ± 0.193 132i, 0.602 513 + u_0
			−0.549 331	0.145 871, 0.515 342, 0.497 186 + u_0, 0.847 232 + u_0
			−0.345 969	0.136 943, 0.431 537 + u_0, 0.671 367 + u_0, 1.101 + u_0
			0.259 969	0.506 611 + u_0, 0.871 82 + u_0, 0.160 443 ± 0.150 348i
			0.842 045	0.287 219, 0.297 174 ± 0.310 653i, 0.609 213 + u_0
			0.891 361	0.497 959 + u_0, 0.849 881 + u_0, 0.370 167 ± 0.118 987i
			0.948 984	0.285 065, 0.429 407 + u_0, 0.668 011 + u_0, 1.094 95 + u_0
			1.193 4	0.429 338 ± 0.160 247i, 0.373 211 ± 0.475 013i
			1.338 34	0.569 12, 0.582 163 + u_0, 0.533 392 ± 0.368 923i
			1.485 84	0.481 42 + u_0, 0.807 965 + u_0, 0.649 061 ± 0.215 203i
			1.647 07	0.733 488, 0.416 86 + u_0, 0.647 858 + u_0, 1.054 04 + u_0
			1.822 55	0.367 461 + u_0, 0.570 419 + u_0, 0.839 668 + u_0, 1.291 77 + u_0

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 (1.4) 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 $\tilde{u} = 0.690\,849 + 1.570\,8\mathrm{i}$ which corresponds to the (single) transfer matrix eigenvalue, but also an additional solution of the Bethe Ansatz equation $\tilde{u} = 1.4208\mathrm{i}$ 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.

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

N	k	M	Ground-state energy E	Shifted Bethe roots $\tilde{u}_j$
1	0	0	−2.794 13	–
2	1	1	−1.577 15	0.094 445 5
3	0	1	−4.582 16	0.097 325 2
4	1	2	−3.347 7	0.055 945 2, 0.139 137
5	0	2	−6.351 77	0.057 297 2, 0.141 22
6	1	3	−5.108 16	0.040 297 8, 0.089 333 4, 0.168 789
7	0	3	−8.111 81	0.041 060 5, 0.090 660 2, 0.170 368

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)[8].

2.4. Massive regime

For the case that η 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

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

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.

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

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 $\mathrm{Re}\,\tilde{u}_j > 0$ and $-\frac{\pi}{2} < \mathrm{Im}\,\tilde{u}_j \leqslant \frac{\pi}{2}$; or $\mathrm{Re}\,\tilde{u}_j = 0$ and $0 < \mathrm{Im}\,\tilde{u}_j \leqslant \frac{\pi}{2}$.

N	k	M	E	Shifted Bethe roots $\tilde{u}_j$
0	1	0	0.282 16	–
1	2	1	−0.478 182	0.274 302i
			0.478 182	1.822 87 + u_0
2	3	2	−1.528 36	0.123 806i, 1.834 83 + u_0
			0.128 052	0.184 296 ± 0.327 865i
			0.496 614	0.460 762i, 1.849 61 + u_0
			0.903 692	1.444 53 + u_0, 2.250 6 + u_0
3	4	3	−2.273 3	0.086 6767i, 0.369 644i, 1.874 89 + u_0
			−1.809 33	0.079 402 4i, 1.453 56 + u_0, 2.270 91 + u_0
			−0.009 285 35	0.140 292 ± 0.238 892i, 1.869 94 + u_0
			−0.004 632 36	0.210 583i, 1.454 52 + u_0, 2.272 83 + u_0
			0.684 253	0.387 332i, 0.337 297 ± 0.355 183i
			0.903 368	0.202 474 ± 0.507 083i, 1.897 23 + u_0
			1.127 43	0.608 104i, 1.462 45 + u_0, 2.287 76 + u_0
			1.381 49	1.362 48 + u_0, 1.784 47 + u_0, 2.599 88 + u_0
4	5	4	−3.301 64	0.065 708 7i, 0.173 726i, 1.473 29 + u_0, 2.314 03 + u_0
			−2.219 69	0.064 181 4i, 0.192 461 ± 0.388 014i, 1.943 46 + u_0
			−1.953 89	0.060 966 9i, 0.524 409i, 1.479 97 + u_0, 2.325 36 + u_0
			−1.662 52	0.058 730 6i, 1.365 91 + u_0, 1.799 91 + u_0, 2.626 53 + u_0
			−0.684 81	0.191 746 ± 0.362 798i, 0.163 232i, 1.942 39 + u_0
			−0.565 79	0.146 007i, 0.513 987i, 1.480 2 + u_0, 2.325 76 + u_0
			−0.355 209	0.137 034i, 1.365 99 + u_0, 1.800 22 + u_0, 2.627 01 + u_0
			0.270 674	0.150 351 ± 0.160 618i, 1.472 52 + u_0, 2.312 69 + u_0
			0.872 54	0.310 225 ± 0.295 283i, 0.285 824i, 1.931 76 + u_0
			0.920 906	0.119 052 ± 0.370 73i, 1.479 31 + u_0, 2.324 48 + u_0
			0.978 875	0.285 415i, 1.366 33 + u_0, 1.801 48 + u_0, 2.628 91 + u_0
			1.222 16	0.158 173 ± 0.414 71i, 0.468 95 ± 0.3645 85i
			1.380 81	0.366 909 ± 0.533 061 1i, 0.565 907i, 1.974 05 + u_0
			1.529 04	0.212 615 ± 0.654 327i, 1.494 36 + u_0, 2.348 75 + u_0
			1.687 84	0.724 014i, 1.368 69 + u_0, 1.809 52 + u_0, 2.640 55 + u_0
			1.880 7	1.350 68 + u_0, 1.669 25 + u_0, 2.100 24 + u_0, 2.919 17 + u_0

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

N	k	M	Ground-state energy E	Shifted Bethe roots $\tilde{u}_j$
1	0	0	−2.864 59	–
2	1	1	−1.616 48	0.094 105 8i
3	0	1	−4.713 23	0.096 971 3i
4	1	2	−3.443 2	0.055 849 2i, 0.138 676i
5	0	2	−6.538 87	0.057 197 3i, 0.140 752i

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

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

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

N	k	M	E	Shifted Bethe roots $\tilde{u}_j$
1	0	0	0	–
3	0	1	−2.063 61	0.081 128 7
			−0.202 938	0.228 372
			0.983 167	1.177 9 + u_0
			1.283 38	0.567 083i
5	0	2	−3.932 43	0.051 837 3, 0.121 304
			−2.558 68	0.050 152 1, 0.259 987
			−1.618 87	0.047 091 1, 1.182 04 + u_0
			−1.536 27	0.114 268, 0.255 101
			−1.347 1	0.045 259 9, 0.570 638i
			−0.687 493	0.104 34, 1.180 27 + u_0
			−0.474 743	0.099 198 8, 0.568 57i
			0.268 219	0.119 246 ± 0.149 991i
			0.486 895	0.193 28, 1.174 89 + u_0
			0.642 915	0.178 75, 0.564 459i
			0.954 064	0.278 324 ± 0.155 511i
			1.498 74	0.407 709, 1.148 97 + u_0
			1.658 95	0.347 419, 0.557 976i
			1.969 38	0.850 516 + u_0, 1.625 72 + u_0
			2.281 62	0.551 706i, 1.243 28 + u_0
			2.394 8	0.550 319i, 0.950 981i

We first argue that for this case all the energy eigenvalues are two-fold degenerate. Indeed, it is easy to see that the Hamiltonian commutes with the operator U defined by[9]

$$U = CP \tag{3.2}$$

where C is the 'charge conjugation' operator

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

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

$$P\sigma_n^j P = \sigma_{N+1-n}^j \tag{3.4}$$

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 ± 1. For N odd, U has an equal number of +1 and -1 eigenvalues[10]. It follows that all energy eigenvalues are two-fold degenerate. In fact, since U commutes with the full transfer matrix $t(u)$, all the eigenvalues $\Lambda(u)$ are two-fold degenerate.

[9] 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.

[10] 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,

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

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

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

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

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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