Discrete symmetries and *S*-matrix of the *XXZ* chain

LETTER TO THE EDITOR

Discrete symmetries and S-matrix of the XXZ chain

Anastasia Doikou and Rafael I Nepomechie

Physics Department, PO Box 248046, University of Miami, Coral Gables, FL 33124, USA

Abstract. We formulate the notion of parity for the periodic XXZ spin chain within the quantum inverse scattering method. We also propose an expression for the eigenvalues of the charge conjugation operator. We use these discrete symmetries to help classify low-lying $S^z = 0$ states in the critical regime, and we give a direct computation of the S-matrix.

1. Introduction and summary

The periodic anisotropic Heisenberg (or 'XXZ') spin chain, with the Hamiltonian

$$H = \tfrac{1}{4} \sum_{n=1}^{N} \{\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \Delta(\sigma_n^z \sigma_{n+1}^z - 1)\} \qquad \boldsymbol{\sigma}_{N+1} \equiv \boldsymbol{\sigma}_1 \qquad (1)$$

has a long and rich history [1–14]. It is the prototype of all integrable models. The development of the quantum inverse scattering method (QISM)/algebraic Bethe ansatz [7] systematized earlier results, and paved the way for far-reaching generalizations.

Parity symmetry has played a valuable role in continuum quantum field theory, including integrable quantum field theory [15]. However, the notion of parity for discrete spin models, in particular for those which are integrable, has not (to our knowledge) been discussed. We show here that parity has a simple realization in the algebraic Bethe ansatz, involving negation of the spectral parameter, i.e. $\lambda \to -\lambda$ (see equation (13) below).

We consider also charge conjugation symmetry [5]. We conjecture that Bethe ansatz states of the XXZ chain with $S^z = 0$ are eigenstates of the charge conjugation operator, with eigenvalues $(-1)^\nu$, where ν is given by equation (17).

Working within the framework of the string hypothesis [4], we use these discrete symmetries to help classify low-lying $S^z = 0$ states [6, 9] in the critical regime with $0 < \Delta < 1$. Moreover, we compute the S-matrix elements corresponding to these states using the method of Korepin [15] and Andrei and Destri [16]. Our results for the S-matrix agree with those obtained by thermodynamic methods [11, 12].

This letter is organized as follows. In section 2, after a brief review of the algebraic Bethe ansatz, we define the parity operator, and we show how it acts on the fundamental quantities of the QISM formalism. We also review the definition of the charge conjugation operator, and we propose an expression for the corresponding eigenvalues. In section 3 we use the root densities for low-lying $S^z = 0$ states in the critical regime to calculate the parity and charge conjugation quantum numbers of these states, as well as the S-matrix. We conclude in section 4 by briefly listing some remaining unanswered questions. A more detailed exposition of these results will be given elsewhere [17].

2. Algebraic Bethe ansatz and discrete symmetries

In order to fix notations, we briefly recall the essential elements of the algebraic Bethe ansatz for the XXZ chain (see the above-cited references for details). We consider the $A_1^{(1)}$ R-matrix

$$
R(\lambda) = \begin{pmatrix} a(\lambda) & & & \\ & b(\lambda) & c & \\ & c & b(\lambda) & \\ & & & a(\lambda) \end{pmatrix} \tag{2}
$$

where

$$
a(\lambda) = \frac{\sinh(\mu(\lambda + \mathrm{i}))}{\sinh(\mathrm{i}\mu)} \qquad b(\lambda) = \frac{\sinh(\mu\lambda)}{\sinh(\mathrm{i}\mu)} \qquad c = 1. \tag{3}
$$

We regard $R(\lambda)$ as an operator acting on the tensor product space $V \otimes V$, where V is a two-dimensional complex vector space. This R-matrix is a solution of the Yang–Baxter equation

$$
R_{12}(\lambda - \lambda') \, R_{13}(\lambda) \, R_{23}(\lambda') = R_{23}(\lambda') \, R_{13}(\lambda) \, R_{12}(\lambda - \lambda') \tag{4}
$$

where R_{ij} are operators on $V \otimes V \otimes V$, with $R_{12} = R \otimes 1$, etc. The L operators $L_{0n}(\lambda) = R_{0n}(\lambda - \frac{\mathrm{i}}{2})$ act on so-called auxiliary (0) and quantum (n) spaces. The monodromy matrix $T_0(\lambda)$ is defined as a product of N such operators

$$
T_0(\lambda) = L_{0N}(\lambda) \dots L_{01}(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}. \tag{5}
$$

The transfer matrix $t(\lambda)$, defined by tracing over the auxiliary space

$$
t(\lambda) = \mathrm{tr}_0 \, T_0(\lambda) = A(\lambda) + D(\lambda) \tag{6}
$$

has the commutativity property $[t(\lambda), t(\lambda')] = 0$. The transfer matrix also commutes with the z component of the total spin, $S^z = \frac{1}{2} \sum_{n=1}^N \sigma_n^z$. The Hamiltonian

$$
H = \frac{\mathrm{i} \sin \mu}{2\mu} \frac{\mathrm{d}}{\mathrm{d}\lambda} \log t(\lambda) \Big|_{\lambda = \frac{\mathrm{i}}{2}} - \frac{N}{2} \cos \mu \tag{7}
$$

coincides with the XXZ Hamiltonian (1), provided $\Delta = \cos \mu$. The critical regime $-1 < \Delta < 1$ corresponds to μ real, with $0 < \mu < \pi$. The momentum operator P is defined by $P = \frac{1}{\mathrm{i}} \log t(\frac{\mathrm{i}}{2})$, since $t(\frac{\mathrm{i}}{2})$ is the one-site shift operator.

Let $\omega_+ = \binom{1}{0}^{\otimes N}$ be the ferromagnetic vacuum vector with all spins up. The Bethe state $\prod_{\alpha=1}^M B(\lambda_\alpha)\omega_+$ is an eigenstate of the transfer matrix $t(\lambda)$ if $\{\lambda_1, \dots, \lambda_M\}$ are distinct and obey the Bethe ansatz equations

$$
\left(\frac{\sinh \mu(\lambda_\alpha + \frac{\mathrm{i}}{2})}{\sinh \mu(\lambda_\alpha - \frac{\mathrm{i}}{2})} \right)^N = \prod_{\substack{\beta=1 \\ \beta \neq \alpha}}^M \frac{\sinh \mu(\lambda_\alpha - \lambda_\beta + \mathrm{i})}{\sinh \mu(\lambda_\alpha - \lambda_\beta - \mathrm{i})} \qquad \alpha = 1, \dots, M. \tag{8}
$$

The corresponding energy and momentum are given by

$$
E = -\sin^2 \mu \sum_{\alpha=1}^M \frac{1}{\cosh(2\mu\lambda_\alpha) - \cos \mu} \qquad P = \frac{1}{\mathrm{i}} \sum_{\alpha=1}^M \log \frac{\sinh \mu(\lambda_\alpha + \frac{\mathrm{i}}{2})}{\sinh \mu(\lambda_\alpha - \frac{\mathrm{i}}{2})} \qquad (\mathrm{mod} \, 2\pi) \tag{9}
$$

and $S^z = \frac{N}{2} - M$.

2.1. Parity

We define the parity operator Π on a ring of N spins by

$$\Pi\, X_n \Pi^{-1} = X_{N+1-n} \tag{10}$$

where X_n is any operator at site $n \in \{1, 2, \ldots, N\}$. Clearly, Π acts on the tensor product space $V^{\otimes N}$. We can represent Π by

$$\Pi = \begin{cases} \mathcal{P}_{1,N}\mathcal{P}_{2,N-1}\ldots\mathcal{P}_{\frac{N}{2},\frac{N+2}{2}} & \text{for } N = \text{even} \\ \mathcal{P}_{1,N}\mathcal{P}_{2,N-1}\ldots\mathcal{P}_{\frac{N-1}{2},\frac{N+3}{2}} & \text{for } N = \text{odd} \end{cases} \tag{11}$$

where $\mathcal{P}_{ij}$ is the permutation matrix which permutes the ith and jth vector spaces. We note that $\Pi = \Pi^{-1} = \Pi^\dagger$ and hence $\Pi\Pi^\dagger = 1$.

The 'parity invariance' of the R-matrix $\mathcal{P}_{12}R_{12}(\lambda)\mathcal{P}_{12} = R_{12}(\lambda)$ implies that the XXZ Hamiltonian is parity invariant, $\Pi H \Pi = H$. Moreover, $\Pi S^z \Pi = S^z$ and $\Pi P \Pi = -P$.

Under parity, the order of the L operators in the monodromy matrix is reversed, $\Pi\, T_0(\lambda)\Pi = L_{01}(\lambda)\ldots L_{0N}(\lambda)$. With the help of the 'time-reversal' invariance of the R-matrix $R_{12}(\lambda)^{t_1 t_2} = R_{12}(\lambda)$ (t_j denotes transposition in the jth space), one can show that

$$\Pi T_0(\lambda)\Pi = (-)^{N-1} W_0 T_0(-\lambda)^{t_0} W_0 \qquad W = i\sigma^y. \tag{12}$$

In particular, we see that $\Pi t(\lambda)\Pi = (-)^N t(-\lambda)$. Evidently, the parity operator does not commute with the transfer matrix. We also obtain from (12) the fundamental result

$$\Pi B(\lambda)\Pi = (-)^{N-1} B(-\lambda). \tag{13}$$

We shall use this result, together with the fact $\Pi\omega_+ = \omega_+$, to investigate whether the eigenvectors of the transfer matrix are also eigenvectors of the parity operator. Since $\{\Pi, P\} = 0$, a Bethe state can be an eigenstate of Π only if the momentum is $P = 0$ or π (mod 2π).

2.2. Charge conjugation

The charge conjugation matrix C is defined (see, e.g. [5]) by $C = \sigma^x$, since it interchanges the two-component spins $\binom{1}{0}$ and $\binom{0}{1}$. We denote by $\mathcal{C}$ the corresponding operator acting on the tensor product space $V^{\otimes N}$,

$$\mathcal{C} = C_1 \ldots C_N. \tag{14}$$

It has the properties $\mathcal{C} = \mathcal{C}^{-1} = \mathcal{C}^\dagger$, and hence $\mathcal{C}\mathcal{C}^\dagger = 1$.

The invariance of the R-matrix under charge conjugation $C_1 C_2 R_{12}(\lambda)C_1 C_2 = R_{12}(\lambda)$ implies that the monodromy matrix obeys

$$\mathcal{C}T_0(\lambda)\mathcal{C} = C_0 T_0(\lambda)C_0. \tag{15}$$

In particular, we see that the transfer matrix is invariant under charge conjugation $\mathcal{C}t(\lambda)\mathcal{C} = t(\lambda)$, while the operator $B(\lambda)$ is mapped to $C(\lambda)$,

$$\mathcal{C}B(\lambda)\mathcal{C} = C(\lambda). \tag{16}$$

Moreover, $\mathcal{C}\omega_+ = \omega_-$, where $\omega_- = \binom{0}{1}^{\otimes N}$ is the ferromagnetic vacuum vector with all spins down.

Since $\{\mathcal{C}, S^z\} = 0$, a Bethe state can be an eigenstate of $\mathcal{C}$ only if $S^z = 0$. This corresponds to $M = N/2$ with N an even integer.

We conjecture that the eigenvectors of the transfer matrix with $M = N/2$ are also eigenvectors of $\mathcal{C}$, with eigenvalues $(-)^\nu$, where

$$\nu = \frac{2i\mu}{\pi} \sum_{\alpha=1}^{N/2} \lambda_\alpha + \frac{N}{2} \qquad (\mathrm{mod}\, 2). \tag{17}$$

This conjecture is supported by explicit checks for $N = 2$ and $N = 4$, and it corresponds to the XXZ limit of a result [5, 6] for the XYZ chain. Unfortunately, Baxter's Q-operator proof of the XYZ result, which relies on the quasidouble-periodicity of certain elliptic functions, does not survive the XXZ limit. (The XYZ result is important, and so it is noteworthy that there does not appear to be a proof of it within the generalized algebraic Bethe ansatz.) Certainly, equation (16) alone does not seem to be sufficiently powerful to investigate this conjecture.

3. Low-lying $S^z = 0$ states

We now examine some low-lying $S^z = 0$ states of the critical XXZ chain within the framework of the string hypothesis [4, 6]. From the so-called root densities, we compute the parity and charge conjugation quantum numbers of these states, and we give a direct computation of the two-particle S-matrix.

3.1. Ground state

For simplicity, we henceforth restrict ourselves to the range $0 < \mu < \frac{\pi}{2}$. The ground state then lies in the sector with N even, and is characterized by $M = N/2$ real roots [3, 4]. A quantity of central importance is the root density $\sigma(\lambda)$, which is defined so that the number of λ_α in the interval $[\lambda, \lambda + d\lambda]$ is $N\sigma(\lambda)\, d\lambda$. The root density for the ground state is given by $\sigma(\lambda) = (2\cosh\pi\lambda)^{-1} \equiv s(\lambda)$.

We now argue that the ground state is a parity eigenstate. Denoting the ground state by $|v\rangle$, we have

$$|v\rangle = \prod_{\alpha=1}^{N/2} B(\lambda_\alpha)\omega_+ = \exp\left(\sum_{\alpha=1}^{N/2} \log B(\lambda_\alpha)\right)\omega_+ = \exp\left(N \int_{-\infty}^{\infty} d\lambda\, \sigma(\lambda) \log B(\lambda)\right)\omega_+. \tag{18}$$

Moreover, using (13), we obtain

$$\Pi|v\rangle = (-)^{N/2} \prod_{\alpha=1}^{N/2} B(-\lambda_\alpha)\omega_+ = (-)^{N/2} \exp\left(N \int_{-\infty}^{\infty} d\lambda\, \sigma(\lambda) \log B(-\lambda)\right)\omega_+$$

$$= (-)^{N/2} \exp\left(N \int_{-\infty}^{\infty} d\lambda\, \sigma(-\lambda) \log B(\lambda)\right)\omega_+ \tag{19}$$

where in passing to the last line we have made the change of variables $\lambda \to -\lambda$. Finally, comparing equations (18) and (19), and using the fact that the root density is an even function $\sigma(-\lambda) = \sigma(\lambda)$, we conclude that

$$\Pi\,|v\rangle = (-)^{N/2}|v\rangle. \tag{20}$$

The nondegeneracy of the ground state implies that this state is also a charge conjugation eigenstate. Formula (17) implies that the corresponding eigenvalue is also $(-)^{N/2}$, since

$$\sum_{\alpha=1}^{N/2} \lambda_\alpha = N \int_{-\infty}^{\infty} d\lambda\, \sigma(\lambda)\lambda = 0 \tag{21}$$

where again we have used the fact that the root density is an even function.

3.2. Two-particle excited states

There are two distinct two-particle states with $S^z = 0$ (again with N even and $M = N/2$) [6, 9] which are distinguished by their parity and charge conjugation quantum numbers. The first state, which we label by (a), is the two-hole state with one string of length 2 (i.e a pair of roots of the form $\lambda_0 \pm \frac{i}{2}$, with λ_0 real) and all other roots real. The corresponding density is given by

$$\sigma_{(a)}(\lambda) = s(\lambda) + \frac{1}{N}\left[\sum_{\alpha=1}^{2} J(\lambda - \tilde{\lambda}_\alpha) - a_1(\lambda - \lambda_0; \mu')\right] \tag{22}$$

where

$$J(\lambda) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, e^{-i\omega\lambda}\frac{\sinh((\frac{\pi}{\mu} - 2)\frac{\omega}{2}))}{2\sinh((\frac{\pi}{\mu} - 1)\frac{\omega}{2})\cosh(\frac{\omega}{2})} \qquad a_1(\lambda; \mu) = \frac{\mu}{\pi}\frac{\sin\mu}{\cosh(2\mu\lambda) - \cos\mu} \tag{23}$$

and μ' is the 'renormalized' anisotropy parameter given by $\mu' = \pi\mu/(\pi - \mu)$. Moreover, $\{\tilde{\lambda}_\alpha\}$ are the hole rapidities, and the centre of the 2-string is given by $\lambda_0 = (\tilde{\lambda}_1 + \tilde{\lambda}_2)/2$.

Since the density $\sigma_{(a)}(\lambda)$ is not an even function of λ for generic values of $\{\tilde{\lambda}_\alpha\}$, a generalization of the argument (18)–(20) implies that this state is not a parity eigenstate. However, in the 'rest frame' [15]

$$\tilde{\lambda}_1 + \tilde{\lambda}_2 = 0 \tag{24}$$

the density is an even function, and therefore the state is a parity eigenstate, with parity $(-)^{N/2}$. One can verify that in the rest frame the momentum is $P = 0$ or $\pi \pmod{2\pi}$, which is consistent with the fact $\{\Pi, P\} = 0$.

According to our conjecture, this state is an eigenstate of charge conjugation for all values of $\{\tilde{\lambda}_\alpha\}$, with eigenvalue given by formula (17). Remarkably, the first term of that formula gives a vanishing contribution. We conclude that the charge conjugation eigenvalue for this state is also $(-)^{N/2}$.

We consider now the second $S^z = 0$ two-particle state, which we label by (b). This is the two-hole state with one 'negative-parity' string of length 1 (i.e. a root of the form $\lambda_0 + \frac{i\pi}{2\mu}$, with λ_0 real) [4] and all other roots real. The density is given by

$$\sigma_{(b)}(\lambda) = s(\lambda) + \frac{1}{N}\left[\sum_{\alpha=1}^{2} J(\lambda - \tilde{\lambda}_\alpha) - b_1(\lambda - \lambda_0; \mu')\right] \tag{25}$$

where $b_1(\lambda; \mu) = a_1(\lambda + \frac{\pi}{2\mu}; \mu)$, and again $\lambda_0 = (\tilde{\lambda}_1 + \tilde{\lambda}_2)/2$.

As in case (a), this state is not a parity eigenstate for generic values of $\{\tilde{\lambda}_\alpha\}$. Let us now restrict ourselves to the rest frame (24). The Bethe vector is then given by $|v\rangle = B(\frac{i\pi}{2\mu})\prod_{\alpha=1}^{\frac{N}{2}-1} B(\lambda_\alpha)\omega_+$. Acting with the parity operator using equation (13), we obtain

$$\Pi|v\rangle = (-)^{N/2}B\left(-\frac{i\pi}{2\mu}\right)\prod_{\alpha=1}^{\frac{N}{2}-1} B(-\lambda_\alpha)\omega_+$$

$$= -(-)^{N/2}B\left(\frac{i\pi}{2\mu}\right)\prod_{\alpha=1}^{\frac{N}{2}-1} B(-\lambda_\alpha)\omega_+$$

$$= -(-)^{N/2}|v\rangle. \tag{26}$$

In passing to the second line, we have used the quasiperiodicity property $B(\lambda \pm \frac{\mathrm{i}\pi}{\mu}) = (-)^{N+1}B(\lambda)$, and to arrive at the last line we use the fact that (in the rest frame) the density is an even function of λ. Thus, the state has parity $-(-)^{N/2}$.

Unlike case (a), here the first term of formula (17) for the charge conjugation eigenvalue does give a contribution, namely, -1. We conclude that the charge conjugation eigenvalue for this state is also $-(-)^{N/2}$.

We recall that a boson–antiboson state with a symmetric (antisymmetric) wavefunction has positive (negative) Π and $\mathcal{C}$, while for a fermion–antifermion state the opposite is true (see, e.g. [18, 19].) Evidently the statistics of the XXZ excitations vary with the value of N.

3.3. S-matrix

We define the S-matrix $S(\tilde{\lambda}_1, \tilde{\lambda}_2)$ by the momentum quantization condition [15, 16]

$$(\mathrm{e}^{\mathrm{i}p(\tilde{\lambda}_1)N}S(\tilde{\lambda}_1, \tilde{\lambda}_2) - 1)|\tilde{\lambda}_1, \tilde{\lambda}_2\rangle = 0 \tag{27}$$

where $\tilde{\lambda}_1$, $\tilde{\lambda}_2$ are the hole rapidities, and $p(\lambda)$ is the hole momentum. The S matrix eigenvalues are given (up to a rapidity-independent phase factor) by

$$S_{(j)} \sim \exp\left\{\mathrm{i}2\pi N \int_{-\infty}^{\tilde{\lambda}_1} (\sigma_{(j)}(\lambda) - s(\lambda))\,\mathrm{d}\lambda\right\} \qquad j = a, b \tag{28}$$

where $S_{(a)}$ and $S_{(b)}$ are the eigenvalues of the S-matrix corresponding to states (a) and (b), respectively.

Recalling expressions (22), (25) for the root densities, it is clear that the S-matrix eigenvalues have the common factor

$$
\begin{aligned}
S_{(0)} &= \exp\left\{\mathrm{i}2\pi \sum_{\alpha=1}^{2} \int_{-\infty}^{\tilde{\lambda}_1} J(\lambda - \tilde{\lambda}_\alpha)\,\mathrm{d}\lambda\right\} \\
&= \exp\left\{\int_0^\infty \frac{\mathrm{d}\omega}{\omega} \frac{\sinh((\frac{\pi}{2\mu'} - \frac{1}{2})\omega)\sinh(\mathrm{i}\omega\tilde{\lambda})}{\sinh(\frac{\pi\omega}{2\mu'})\cosh(\frac{\omega}{2})}\right\} \\
&= \prod_{n=0}^{\infty}\left\{\frac{\Gamma[(1 + \frac{\pi}{\mu'}n - \mathrm{i}\tilde{\lambda})/2]\,\Gamma[(2 + \frac{\pi}{\mu'}n + \mathrm{i}\tilde{\lambda})/2]}{\Gamma[(1 + \frac{\pi}{\mu'}n + \mathrm{i}\tilde{\lambda})/2]\,\Gamma[(2 + \frac{\pi}{\mu'}n - \mathrm{i}\tilde{\lambda})/2]}\right. \\
&\quad \left. \times \frac{\Gamma[(\frac{\pi}{\mu'}(n+1) + \mathrm{i}\tilde{\lambda})/2]\,\Gamma[(1 + \frac{\pi}{\mu'}(n+1) - \mathrm{i}\tilde{\lambda})/2]}{\Gamma[(\frac{\pi}{\mu'}(n+1) - \mathrm{i}\tilde{\lambda})/2]\,\Gamma[(1 + \frac{\pi}{\mu'}(n+1) + \mathrm{i}\tilde{\lambda})/2]}\right\}
\end{aligned} \tag{29}
$$

where $\tilde{\lambda} = \tilde{\lambda}_1 - \tilde{\lambda}_2$. Moreover, we obtain (up to a rapidity-independent phase factor)

$$S_{(a)} = S_{(0)} \frac{\sinh(\mu'(\tilde{\lambda} + \mathrm{i})/2)}{\sinh(\mu'(\tilde{\lambda} - \mathrm{i})/2)} \qquad S_{(b)} = S_{(0)} \frac{\cosh(\mu'(\tilde{\lambda} + \mathrm{i})/2)}{\cosh(\mu'(\tilde{\lambda} - \mathrm{i})/2)}. \tag{30}$$

This coincides with the S-matrix of sine-Gordon/massive Thirring model [15, 20, 21], provided we identify the sine-Gordon coupling constant as $\beta^2 = 8(\pi - \mu)$. This result has been obtained for the XXZ chain previously, although by less direct means, in [11, 12]. Note that the regime $0 < \mu < \frac{\pi}{2}$ in which we work corresponds to the 'repulsive' regime $4\pi < \beta^2 < 8\pi$.

4. Outlook

A number of issues remain to be explored. It would be interesting to find a proof (or counterexample!) of formula (17) for the charge conjugation eigenvalues of the Bethe ansatz states. It may be worthwhile investigating discrete symmetries in integrable chains constructed with higher-rank R-matrices, [22, 23] such as $A_{\mathcal{N}-1}^{(1)}$ with $\mathcal{N} > 2$. Since these R-matrices are not parity invariant, neither are the corresponding Hamiltonians. However, the R-matrices do have PT symmetry, which may lead to a useful symmetry on the space of states. Moreover, we have not discussed here the interesting case of the noncritical ($\Delta > 1$) regime [24].

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