Parity and Charge Conjugation Symmetries and $S$ Matrix of the XXZ Chain

Anastasia Doikou and Rafael I. Nepomechie

Physics Department, P.O. 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

\[ H = \frac{1}{4} \sum_{n=1}^{N} \left\{ \sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \Delta \left( \sigma_n^z \sigma_{n+1}^z - 1 \right) \right\}, \quad \vec{\sigma}_{N+1} \equiv \vec{\sigma}_1, \]  

(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. (See, e.g., [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., \( \lambda \rightarrow -\lambda \). (See Eq. (35) 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 \( \nu \) is given by Eq. (52).

Working within the framework of the string hypothesis [4], we use these discrete symmetries to help classify low-lying \( S^z = 0 \) states [3, 4] 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-Destri [16]. Our results for the \( S \) matrix agree with those obtained by thermodynamic methods [11], [12].

The outline of this paper is 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 compute root densities for low-lying states in the critical regime. We use these densities to calculate quantum numbers – in particular, parity and charge conjugation – of the \( S^z = 0 \) states, as well as the \( S \) matrix. We conclude in Section 4 by briefly listing some remaining unanswered questions. This paper is an expanded version of a recent letter [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 \( A_1^{(1)} \)
\[ R(\lambda) = \begin{pmatrix} a(\lambda) & b(\lambda) & c \\ c & b(\lambda) & a(\lambda) \end{pmatrix}, \]

where

\[ a(\lambda) = \frac{\sinh(\mu(\lambda + i))}{\sinh(i\mu)} \]

\[ b(\lambda) = \frac{\sinh(\mu\lambda)}{\sinh(i\mu)} \]

\[ c = 1. \]

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

\[ R_{12}(\lambda - \lambda') R_{13}(\lambda') R_{23}(\lambda') = R_{23}(\lambda') R_{13}(\lambda) R_{12}(\lambda - \lambda'), \]

where \( R_{ij} \) are operators on \( V \otimes V \otimes V \), with \( R_{12} = R \otimes 1 \), etc. We define the \( L \) operators

\[ L_{0n}(\lambda) = R_{0n}(\lambda - \frac{i}{2}) = \begin{pmatrix} \alpha_n(\lambda) & \beta_n \\ \gamma_n & \delta_n(\lambda) \end{pmatrix}, \]

which act on so-called auxiliary (0) and quantum (\( n \)) spaces. Evidently,

\[ \alpha(\lambda) = \begin{pmatrix} a(\lambda - \frac{i}{2}) & 0 \\ 0 & b(\lambda - \frac{i}{2}) \end{pmatrix}, \quad \beta = \begin{pmatrix} 0 & 0 \\ 0 & c \end{pmatrix}, \]

\[ \gamma = \begin{pmatrix} 0 & c \\ 0 & 0 \end{pmatrix}, \quad \delta(\lambda) = \begin{pmatrix} b(\lambda - \frac{i}{2}) & 0 \\ 0 & a(\lambda - \frac{i}{2}) \end{pmatrix}. \]

The monodromy matrix \( T_0(\lambda) \) is defined as a product of \( N \) such operators

\[ T_0(\lambda) = L_{0N}(\lambda) \cdots L_{01}(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}. \]

(As is customary, we often suppress the quantum-space subscripts.) It obeys the fundamental relation

\[ R_{12}(\lambda - \lambda') T_1(\lambda) T_2(\lambda') = T_2(\lambda') T_1(\lambda) R_{12}(\lambda - \lambda'). \]
The transfer matrix $t(\lambda)$, defined by tracing over the auxiliary space
\[ t(\lambda) = \text{tr}_0 T_0(\lambda) = A(\lambda) + D(\lambda), \] (9)
has the commutativity property
\[ [t(\lambda), t(\lambda')] = 0 \] (10)
by virtue of the fundamental relation (8). The transfer matrix also commutes with the $z$ component of the total spin,
\[ [t(\lambda), S^z] = 0, \quad S^z = \frac{1}{2} \sum_{n=1}^{N} \sigma^z_n. \] (11)

The Hamiltonian
\[
H = \left. \frac{i \sin \mu}{2 \mu} d \log t(\lambda) \right|_{\lambda = \frac{i}{2}} - \frac{N}{2} \cos \mu \\
= \sum_{n=1}^{N-1} H_{n,n+1} + H_{N,1}, \quad H_{ij} = \frac{i \sin \mu}{2 \mu} P_{ij} R_{ij}(0) - \frac{1}{2} \cos \mu
\]
(12)
coincides with the XXZ Hamiltonian (I), provided
\[ \Delta = \cos \mu. \] (13)

The critical regime $-1 < \Delta < 1$ corresponds to $\mu$ real, with $0 < \mu < \pi$. The momentum operator $P$ is defined by
\[ P = \frac{1}{i} \log t\left(\frac{i}{2}\right), \] (14)
since $t\left(\frac{i}{2}\right)$ is the one-site shift operator.

Let $\omega_+$ be the ferromagnetic vacuum vector with all spins up,
\[ \omega_+ = \left(\begin{array}{c} 1 \\ 0 \end{array} \right) \otimes \cdots \otimes \left(\begin{array}{c} 1 \\ 0 \end{array} \right), \] (15)
which is annihilated by $C(\lambda)$. The operators $B(\lambda)$, which commute among themselves,
\[ [B(\lambda), B(\lambda')] = 0, \] (16)
act as creation operators. The Bethe state
\[ B(\lambda_1) \cdots B(\lambda_M) \omega_+ \] (17)
is an eigenstate of the transfer matrix \( t(\lambda) \), with eigenvalue

\[
\Lambda(\lambda) = \left( \frac{\sinh \mu(\lambda + \frac{i}{2})}{\sinh \mu i} \right)^N \prod_{\alpha=1}^{M} \frac{\sinh \mu (\lambda - \lambda_\alpha - i)}{\sinh \mu (\lambda - \lambda_\alpha)} + \left( \frac{\sinh \mu(\lambda - \frac{i}{2})}{\sinh \mu i} \right)^N \prod_{\alpha=1}^{M} \frac{\sinh \mu (\lambda - \lambda_\alpha + i)}{\sinh \mu (\lambda - \lambda_\alpha)},
\]

if \( \{\lambda_1, \ldots, \lambda_M\} \) are distinct and obey the Bethe Ansatz equations

\[
\left( \frac{\sinh \mu (\lambda_\alpha + \frac{i}{2})}{\sinh \mu (\lambda_\alpha - \frac{i}{2})} \right)^N = \prod_{\beta=1}^{M} \frac{\sinh \mu (\lambda_\alpha - \lambda_\beta + i)}{\sinh \mu (\lambda_\alpha - \lambda_\beta - i)}, \quad \alpha = 1, \ldots, M.
\]

In particular, the energy and momentum are given by

\[
E = -\sin^2 \mu \sum_{\alpha=1}^{M} \frac{1}{\cosh(2\mu \lambda_\alpha) - \cos \mu},
\]

\[
P = \frac{1}{i} \sum_{\alpha=1}^{M} \log \left( \frac{\sinh \mu (\lambda_\alpha + \frac{i}{2})}{\sinh \mu (\lambda_\alpha - \frac{i}{2})} \right) \pmod{2\pi}.
\]

The vector \( |\Phi\rangle \) is also an eigenvector of \( S^z \) with eigenvalue

\[
S^z = \frac{N}{2} - M.
\]

Having reviewed the QISM description of the XXZ model, we now consider some of its discrete symmetries.

### 2.1 Parity

We define the parity operator \( \Pi \) on a ring of \( N \) spins by

\[
\Pi X_n \Pi^{-1} = X_{N+1-n},
\]

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

\[
\Pi = \left\{ \begin{array}{ll}
P_{1,N} P_{2,N-1} \cdots P_{N-1,2} & \text{for } N = \text{even} \\
P_{1,N} P_{2,N-1} \cdots P_{N-1,2} & \text{for } N = \text{odd} \\
\end{array} \right.
\]

where \( P_{ij} \) is the permutation matrix which permutes the \( i^{th} \) and \( j^{th} \) vector spaces. We note that \( \Pi = \Pi^{-1} = \Pi^\dagger \) and hence \( \Pi \Pi^\dagger = 1 \).
It is easy to see that both the Hamiltonian \( H \) and the spin \( S^z \) are invariant under parity, while the momentum \( P \) changes sign

\[
\Pi H \Pi = H, \quad \Pi S^z \Pi = S^z, \quad \Pi P \Pi = -P.
\]

(24)

Indeed, the “parity invariance” of the \( R \) matrix

\[
R_{12} \frac{t(\lambda)}{2} R_{12} = R_{12}(\lambda)
\]

(25)

implies that the two-site Hamiltonian \( H_{12} \) satisfies

\[
\mathcal{P}_{ij} H_{ij} \mathcal{P}_{ij} = H_{ij},
\]

(26)

and hence the full Hamiltonian is parity invariant. Moreover, for any \( X_n \), we have the chain of equalities

\[
\Pi t(\frac{i}{2}) X_n t(\frac{i}{2})^{-1} \Pi = \Pi X_{n+1} \Pi = X_{N-n} = t(\frac{i}{2})^{-1} X_{N+1-n} t(\frac{i}{2}) = t(\frac{i}{2})^{-1} \Pi X_n \Pi t(\frac{i}{2}),
\]

(27)

which is consistent with \( \Pi t(\frac{i}{2}) \Pi = t(\frac{i}{2})^{-1} \), implying the third relation in Eq. (24).

In order to go further, we must investigate the behavior of the monodromy matrix under parity. To this end, we first note the “time-reversal” invariance of the \( R \) matrix

\[
R_{12}(\lambda) t_1 t_2 = R_{12}(\lambda),
\]

(28)

where \( t_j \) denotes transposition in the \( j^{th} \) space, which implies the identity

\[
L_{0n}(\lambda)^{t_2} = L_{0n}(\lambda)^{t_n};
\]

(29)

and we observe that

\[
\alpha_n(-\lambda) = -\delta_n(\lambda),
\]

(30)

from which it follows that

\[
L_{0n}(\lambda)^{t_n} = W_0 L_{0n}(-\lambda) W_0, \quad W = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.
\]

(31)

We next observe that

\[
T_0(\lambda)^{t_2} = L_{01}(\lambda)t_0 \cdots L_{0N}(\lambda)^{t_0} = L_{01}(\lambda)^{t_1} \cdots L_{0N}(\lambda)^{t_N} = W_0 L_{01}(-\lambda) W_0 \cdots W_0 L_{0N}(-\lambda) W_0 = (-)^{N-1} W_0 L_{01}(-\lambda) \cdots L_{0N}(-\lambda) W_0,
\]

(32)
where the second line uses (29), the third line uses (31), and the last line uses $W^2 = -1$. Finally, we obtain the desired result

$$
\Pi T_0(\lambda) \Pi = \Pi L_{0N}(\lambda) \Pi \cdots \Pi L_{01}(\lambda) \Pi
= L_{01}(\lambda) \cdots L_{0N}(\lambda)
= (-)^{N-1} W_0 T_0(-\lambda)^t W_0.
$$

(33)

Note that under parity, the order of the $L$ operators in the monodromy matrix is reversed.

In particular, we see that

$$
\Pi t(\lambda) \Pi = (-)^N t(-\lambda).
$$

(34)

Evidently, the parity operator does not commute with the transfer matrix. Nevertheless, if $|v\rangle$ is an eigenvector of $t(\lambda)$ with eigenvalue $\Lambda(\lambda)$, then $\Pi |v\rangle$ is also an eigenvector of $t(\lambda)$, but with eigenvalue $(-)^N \Lambda(-\lambda)$.

We also obtain from (33) the fundamental result

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

(35)

We shall use this result, together with the fact

$$
\Pi \omega_+ = \omega_+,
$$

(36)

to investigate whether the eigenvectors of the transfer matrix are also eigenvectors of the parity operator. Eqs. (24), (34) and (35) are the key results of this subsection.

We conclude this subsection with a few general observations. We first note that if the set $\{\lambda_\alpha\}$ is a solution of the Bethe Ansatz equations, then so is the corresponding set $\{-\lambda_\alpha\}$ with each root negated. As always, we assume that the Bethe Ansatz roots are distinct. Moreover, for simplicity, let us assume (in this paragraph) that $N$ is even, and that the roots are nonzero and are not equal to $\frac{i\pi}{2\mu}$. For $M$ even, all the roots can be “paired” $\{\lambda_\alpha\} = \{\lambda_1, -\lambda_1, \ldots, \lambda_M, -\lambda_M\}$, in which case $\{-\lambda_\alpha\}$ is the same set. Eq. (35) then implies that the corresponding state $\Pi_{\alpha=1}^M B(\lambda_\alpha) \omega_+$ is a parity eigenstate, with eigenvalue $(-)^M$. Similarly, a nondegenerate state must have parity $(-)^M$.

There can be Bethe states which are not parity eigenstates. For such cases, the vectors $\Pi_\alpha B(\lambda_\alpha) \omega_+$ and $\Pi_\alpha B(-\lambda_\alpha) \omega_+$ are distinct and are degenerate in energy.

Since $\{\Pi, P\} = 0$, a Bethe state can be an eigenstate of $\Pi$ only if the momentum is $P = 0$ or $\pi \pmod{2\pi}$. 
2.2 Quasi-periodicity

The transfer matrix $t(\lambda)$ and the operators $B(\lambda)$ also satisfy quasi-periodicity conditions, which we now derive. The starting point is the observation

\[
\alpha_n(\lambda \pm \frac{i\pi}{\mu}) = -\alpha_n(\lambda),
\]

\[
\delta_n(\lambda \pm \frac{i\pi}{\mu}) = -\delta_n(\lambda),
\]

(37)

from which it follows that

\[
L_{0n}(\lambda \pm \frac{i\pi}{\mu}) = -S_0 \ L_{0n}(\lambda) \ S_0, \quad S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\]

(38)

We conclude that

\[
T_0(\lambda \pm \frac{i\pi}{\mu}) = (-)^N S_0 \ T_0(\lambda) \ S_0.
\]

(39)

In particular, we obtain the desired quasi-periodicity relations

\[
t(\lambda \pm \frac{i\pi}{\mu}) = (-)^N \ t(\lambda)
\]

(40)

and

\[
B(\lambda \pm \frac{i\pi}{\mu}) = (-)^{N+1} \ B(\lambda).
\]

(41)

We shall make use of the latter relation when computing the parity of certain states.

2.3 Charge conjugation

The charge conjugation matrix $C$ is defined (see, e.g., [5]) by

\[
C = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},
\]

(42)

since it interchanges the two-component spins $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$. We denote by $C$ the corresponding operator acting on the tensor product space $V^\otimes N$,

\[
C = C_1 \cdots C_N.
\]

(43)

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

\footnote{The charge conjugation matrix should not be confused with the element $C(\lambda)$ of the monodromy matrix!}
The invariance of the $R$ matrix under charge conjugation

$$C_1 \ C_2 \ R_{12}(\lambda) \ C_1 \ C_2 = R_{12}(\lambda) \quad (44)$$

implies that the $L$ operators obey

$$C_n \ L_{0n}(\lambda) \ C_n = C_0 \ L_{0n}(\lambda) \ C_0 \quad . \quad (45)$$

It follows that the monodromy matrix obeys

$$\mathcal{C} \ T_0(\lambda) \ \mathcal{C} = C_0 \ T_0(\lambda) \ C_0 \quad . \quad (46)$$

In particular, we see that the transfer matrix is invariant under charge conjugation

$$\mathcal{C} \ t(\lambda) \ \mathcal{C} = t(\lambda) \quad , \quad (47)$$

while the operator $B(\lambda)$ is mapped to $C(\lambda)$,

$$\mathcal{C} \ B(\lambda) \ \mathcal{C} = C(\lambda) \quad . \quad (48)$$

Moreover,

$$\mathcal{C} \ \omega_+ = \omega_- \quad , \quad (49)$$

where $\omega_-$ is the ferromagnetic vacuum vector with all spins down,

$$\omega_- = \left( \begin{array}{l} 0 \\ 1 \end{array} \right) \otimes \cdots \otimes \left( \begin{array}{l} 0 \\ 1 \end{array} \right) \quad . \quad (50)$$

Since $C \sigma^z C = -\sigma^z$, the $z$-component of total spin changes sign under charge conjugation,

$$\mathcal{C} \ S^z \ \mathcal{C} = -S^z \quad . \quad (51)$$

Therefore, a Bethe state can be an eigenstate of $\mathcal{C}$ only if $S^z = 0$. From Eq. (21), we see that this corresponds to $M = N/2$ with $N$ an even integer.

We conjecture that the eigenvectors (17) of the transfer matrix with $M = N/2$ are also eigenvectors of $\mathcal{C}$, with eigenvalues $(-)^\nu$, where

$$\nu = \frac{2i\mu}{\pi} \sum_{\alpha=1}^{N/2} \lambda_\alpha + \frac{N}{2} \quad (\text{mod} \ 2) \quad . \quad (52)$$

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 quasi-double-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, Eqs. (48) and (49) alone do not seem to be sufficiently powerful to investigate this conjecture.
3 Low-lying states

We now examine some low-lying 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 the \(S_z = 0\) states, and we give a direct computation
of the two-particle \(S\) matrix. In the analysis presented below, we find it convenient to work
with the Bethe Ansatz Eqs. (19) in the form

\[
e_1(\lambda_\alpha ; \mu)^N = \prod_{\beta=1}^{M} e_2(\lambda_\alpha - \lambda_\beta ; \mu) , \quad \alpha = 1, \cdots, M , \tag{53}
\]

where

\[
e_n(\lambda ; \mu) = \frac{\sinh \mu (\lambda + \frac{in}{2})}{\sinh \mu (\lambda - \frac{in}{2})} . \tag{54}
\]

3.1 Ground state

For simplicity, we henceforth restrict to the range

\[
0 < \mu < \frac{\pi}{2} . \tag{55}
\]

The ground state then lies in the sector with \(N\) even, and is characterized by \(M = N/2\)
real roots \[3\], \[4\]. We briefly review the procedure for determining the root density, which
describes the distribution of roots in the thermodynamic \((N \to \infty)\) limit. Taking the
logarithm of the Bethe Ansatz Eqs. (53), we obtain

\[
h(\lambda_\alpha) = J_\alpha , \quad \alpha = 1, \cdots, M , \tag{56}
\]

where the so-called counting function \(h(\lambda)\) is given by

\[
h(\lambda) = \frac{1}{2\pi} \left\{ Nq_1(\lambda ; \mu) - \sum_{\beta=1}^{M} q_2(\lambda - \lambda_\beta ; \mu) \right\} , \tag{57}
\]

\(q_n(\lambda ; \mu)\) is an odd function of \(\lambda\) defined by

\[
q_n(\lambda ; \mu) = \pi + i \log e_n(\lambda ; \mu) , \tag{58}
\]

and \(\{J_\alpha\}\) are integers or half-integers lying in a certain range which serve as “quantum
numbers” of the Bethe Ansatz states. The root density \(\sigma(\lambda)\) is defined by

\[
\sigma(\lambda) = \frac{1}{N} \frac{d}{d\lambda} h(\lambda) , \tag{59}
\]
so that the number of $\lambda_\alpha$ in the interval $[\lambda, \lambda + d\lambda]$ is $N\sigma(\lambda)d\lambda$. Passing from the sum in $h(\lambda)$ to an integral, we obtain a linear integral equation for the root density

$$\sigma(\lambda) = a_1(\lambda; \mu) - \int_{-\infty}^{\infty} d\lambda' \sigma(\lambda') a_2(\lambda - \lambda'; \mu),$$

(60)

where

$$a_n(\lambda; \mu) = \frac{1}{2\pi} \frac{d}{d\lambda} q_n(\lambda; \mu) = \frac{\mu}{\pi} \frac{\sin(n\mu)}{\cosh(2\mu\lambda) - \cos(n\mu)}. \quad (61)$$

Solving by Fourier transforms using

$$\hat{a}_n(\omega; \mu) = \frac{\sinh\left(\left(\frac{n\mu}{2} - n\omega\right)\right)}{\sinh\left(\frac{n\omega}{2}\right)} \bigg|_{0 < n < \frac{2\pi}{\mu}},$$

(62)

we conclude that the root density for the ground state is given by

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

(63)

where

$$\hat{s}(\omega) = \frac{\hat{a}_1(\omega; \mu)}{1 + \hat{a}_2(\omega; \mu)} = \frac{1}{2 \cosh\left(\frac{\omega}{2}\right)}. \quad (64)$$

We verify the consistency of this procedure by computing the value of $M$ from the root density:

$$M = \sum_{\alpha=1}^{M} 1 = N \int_{-\infty}^{\infty} d\lambda \ \sigma(\lambda) = N\hat{\sigma}(0) = \frac{N}{2},$$

(65)

and hence, the state indeed has $S^z = 0$. The energy and momentum are

$$E_{gr} = -\pi \sin\mu \sum_{\alpha=1}^{N/2} a_1(\lambda_\alpha) = -\pi \sin\mu \int_{-\infty}^{\infty} d\lambda \ s(\lambda) a_1(\lambda)$$

$$P_{gr} = -\sum_{\alpha=1}^{N/2} [q_1(\lambda_\alpha) - \pi] = \frac{\pi N}{2} \quad (\text{mod } 2\pi). \quad (66)$$

\footnote{Our conventions in the critical regime are

$$\hat{f}(\omega) \equiv \int_{-\infty}^{\infty} e^{i\omega\lambda} f(\lambda) \ d\lambda,$$

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

and we use $*$ to denote the convolution

$$(f * g)(\lambda) = \int_{-\infty}^{\infty} f(\lambda - \lambda') g(\lambda') \ d\lambda'.$$}
The ground state is nondegenerate \[^3\] and therefore, as argued at the end of Section 2.1, this state must be a parity eigenstate with eigenvalue \((-)^{N/2}\). We now give an alternative derivation, in order to illustrate the line of argument which we shall use to compute the parity of excited states. Denoting the ground state by \(|v\rangle\), we have

\[
|v\rangle = \prod_{\alpha=1}^{M} B(\lambda_{\alpha}) \omega_+ = \exp \left( \sum_{\alpha=1}^{M} \log B(\lambda_{\alpha}) \right) \omega_+. \tag{67}
\]

Moreover, using (65), we obtain

\[
\Pi |v\rangle = (-)^{M} \prod_{\alpha=1}^{M} B(-\lambda_{\alpha}) \omega_+ = (-)^{M} \exp \left( N \int_{-\infty}^{\infty} d\lambda \, \sigma(\lambda) \log B(-\lambda) \right) \omega_+. \tag{68}
\]

where in passing to the last line we have made the change of variables \(\lambda \to -\lambda\). Finally, comparing Eqs. (67) and (68), and using the fact that the root density (63) is an even function \(\sigma(-\lambda) = \sigma(\lambda)\), we conclude that

\[
\Pi |v\rangle = (-)^{N/2} |v\rangle. \tag{69}
\]

The nondegeneracy of the ground state also implies that this state is a charge conjugation eigenstate. The formula (52) implies that the corresponding eigenvalue is also \((-)^{N/2}\), since

\[
\sum_{\alpha=1}^{N/2} \lambda_{\alpha} = N \int_{-\infty}^{\infty} d\lambda \, \sigma(\lambda) \lambda = 0, \tag{70}
\]

where again we have made use of the fact that the root density is an even function.

### 3.2 Two-particle excited states

We consider now two-particle excited states, again with \(N\) even. On the basis of the results for the isotropic XXX chain \[^7\], one expects that the particles have \(S^z = \pm 1/2\). Hence, one expects four two-particle excited states: two states with \(S^z = \pm 1\), and two \(S^z = 0\) states which are distinguished by their parity and charge conjugation quantum numbers. Surprisingly, the Bethe Ansatz does not seem to give the \(S^z = \pm 1\) states. Indeed, we find
that the Bethe Ansatz state with two holes and no strings has fractional spin (see Eq. (77) below), which only for $\mu \to 0$ (i.e., the isotropic limit) is equal to 1. We do find two $S^z = 0$ states [6],[9] which indeed are distinguished by their parity and charge conjugation quantum numbers.

(0) Two holes

We consider first the two-hole state with only real roots. We label the holes by the integers or half-integers $\{\tilde{J}_\alpha\}, \alpha = 1,2$. The corresponding hole rapidities $\{\tilde{\lambda}_\alpha\}$ are defined by

$$h(\tilde{\lambda}_\alpha) = \tilde{J}_\alpha, \quad \alpha = 1,2,$$

(71)

where the counting function is given by Eq. (57). We compute the density for this state by the same procedure used for the ground state, except that now in passing from sums to integrals we must take into account the presence of holes, i.e.,

$$\frac{1}{N} \sum_{\alpha=1}^{M} g(\lambda_\alpha) = \int_{-\infty}^{\infty} d\lambda \sigma(\lambda) g(\lambda) - \frac{1}{N} \sum_{\alpha=1}^{2} g(\tilde{\lambda}_\alpha),$$

(72)

for any function $g(\lambda)$. We find

$$\sigma_{(0)}(\lambda) = s(\lambda) + \frac{1}{N} \sum_{\alpha=1}^{2} J(\lambda - \tilde{\lambda}_\alpha),$$

(73)

where

$$\hat{J}(\omega) = \frac{\hat{a}_2(\omega;\mu)}{1 + \hat{a}_2(\omega;\mu)} = \frac{\sinh \left(\left(\frac{\pi}{\mu} - 2\right)\frac{\omega}{2}\right)}{2 \sinh \left(\left(\frac{\pi}{\mu} - 1\right)\frac{\omega}{2}\right) \cosh \left(\frac{\omega}{2}\right)}.$$  

(74)

The energy and momentum are given by

$$E = E_{gr} + \frac{\pi \sin \mu}{\mu} \sum_{\alpha=1}^{2} s(\tilde{\lambda}_\alpha), \quad P = P_{gr} + \sum_{\alpha=1}^{2} p(\tilde{\lambda}_\alpha),$$

(75)

where the hole momentum $p(\lambda) \equiv (q_1 - J* q_1)(\lambda)$ satisfies

$$\frac{d}{d\lambda} p(\lambda) = 2\pi s(\lambda).$$

(76)

We find by a generalization of the computation (65) that this two-particle state has the fractional spin

$$S^z = \frac{\pi}{\pi - \mu},$$

(77)
A similar result has been obtained by thermodynamic arguments \[11\], \[12\]. This result is puzzling for both mathematical and physical reasons: the formula (21) for the spin eigenvalue implies that $S^z$ should be an integer; and as already mentioned, the results for the isotropic XXX chain suggest that this state should have $S^z = 1$, corresponding to two spin $1/2$ particles with spins “up”. A possible resolution is to take in Eq. (72) finite integration limits $\pm \Lambda$ such that

$$\int_{-\Lambda}^{\Lambda} d\lambda \sigma(\lambda) = \frac{1}{2} + \frac{1}{N},$$

which would ensure $S^z = 1$.

We do not attempt to compute the parity of this state, since the value of $M$ is not an integer. Since this state has $S^z \neq 0$, it cannot be an eigenstate of $C$. Indeed, by acting on this state with the charge conjugation operator $C$, one obtains the $S^z = -\frac{\pi}{\pi-\mu}$ state.

(a) Two holes and one 2-string

We consider 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 $\lambda_0$ real) and all other roots real. The Bethe Ansatz Eqs. (53) imply

$$e_1(\lambda_\alpha; \mu)^N = e_1(\lambda_\alpha - \lambda_0; \mu) e_3(\lambda_\alpha - \lambda_0; \mu) \prod_{\beta=1, \beta \neq \alpha}^{M_1^+} e_2(\lambda_\alpha - \lambda_\beta; \mu),$$

$$\alpha = 1, \cdots, M_1^+, \quad (78)$$

$$e_2(\lambda_0; \mu)^N = \prod_{\beta=1}^{M_1^+} e_1(\lambda_0 - \lambda_\beta; \mu) e_3(\lambda_0 - \lambda_\beta; \mu),$$

$$\quad (79)$$

where $M_1^+$ is the number of real roots, i.e., $M = M_1^+ + 2$. The counting function is therefore now given by

$$h(\lambda) = \frac{1}{2\pi} \left\{ N q_1(\lambda; \mu) - \sum_{\beta=1}^{M_1^+} q_2(\lambda - \lambda_\beta; \mu) \right. \left. - [q_1(\lambda - \lambda_0; \mu) + q_3(\lambda - \lambda_0; \mu)] \right\}. \quad (80)$$

Proceeding as in case (0), we find

$$\sigma(a)(\lambda) = s(\lambda) + \frac{1}{N} \left[ \sum_{\alpha=1}^{2} J(\lambda - \tilde{\lambda}_\alpha) - a_1(\lambda - \lambda_0; \mu') \right], \quad (81)$$

This “positive parity” 2-string satisfies the Takahashi-Suzuki conditions for $0 \leq \mu < \pi$.\[13\]
where $\mu'$ is the “renormalized” anisotropy parameter given by

$$\frac{\pi}{\mu'} = \frac{\pi}{\mu} - 1,$$

that is,

$$\mu' = \frac{\pi\mu}{\pi - \mu}.$$

In order to cast the last term in the expression for $\sigma(a)(\lambda)$ as the function $a_1$, it is essential to use $\mu'$ rather than $\mu$.

The center of the 2-string, $\lambda_0$, can be determined from Eq. (79). Taking the logarithm and passing from a sum to an integral, one obtains the condition

$$\sum_{\alpha=1}^{2} q_1(\lambda_0 - \tilde{\lambda}_\alpha; \mu') = 0,$$

which has the solution

$$\lambda_0 = \frac{1}{2} \left( \tilde{\lambda}_1 + \tilde{\lambda}_2 \right).$$

We now investigate the quantum numbers of this state:

- We verify by a generalization of the computation (65) that this state has $S^z = 0$. The energy and momentum are again given by Eq. (75).

- Since the density $\sigma(a)(\lambda)$ is not an even function of $\lambda$ for generic values of $\{\tilde{\lambda}_\alpha\}$, a generalization of the argument (67) - (69) implies that this state is not a parity eigenstate. However, in the “rest frame” [15]

$$\tilde{\lambda}_1 + \tilde{\lambda}_2 = 0,$$

the density is an even function, and therefore the state is a parity eigenstate, with parity $(-)^{N/2}$. We note 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 the conjecture of Section 2.3, this state is an eigenstate of charge conjugation for all values of $\{\tilde{\lambda}_\alpha\}$, with eigenvalue given by the formula (52). Remarkably, the first term of that formula gives a vanishing contribution:

$$\sum_{\alpha=1}^{N/2} \lambda_\alpha = (\lambda_0 + \frac{i}{2}) + (\lambda_0 - \frac{i}{2}) + \sum_{\alpha=1}^{M_1^+} \lambda_\alpha$$
\[ \begin{align*}
&= 2\lambda_0 + N \int_{-\infty}^{\infty} d\lambda \sigma(\lambda) \lambda - \sum_{\alpha=1}^{2} \tilde{\lambda}_\alpha \\
&= N \int_{-\infty}^{\infty} d\lambda \sigma(\lambda) \lambda \\
&= \sum_{\alpha=1}^{2} \int_{-\infty}^{\infty} d\lambda J(\lambda - \tilde{\lambda}_\alpha) \lambda - \int_{-\infty}^{\infty} d\lambda a_1(\lambda - \lambda_0; \mu') \lambda \\
&= \tilde{J}(0) \sum_{\alpha=1}^{2} \tilde{\lambda}_\alpha - \hat{a}_1(0; \mu') \lambda_0 \\
&= 0, \tag{86}
\end{align*} \]

where we have used the relation (84) twice, and also the fact that \( \tilde{J}(\omega) \) and \( \hat{a}_1(\omega; \mu') \) are even functions of \( \omega \), and therefore have a vanishing first derivative at \( \omega = 0 \). We conclude that the charge conjugation eigenvalue for this state is also \( (-)^{N/2} \).

(b) Two holes and one negative-parity 1-string

We now consider 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 \( \lambda_0 \) real) [4] and all other roots real. The Bethe Ansatz Eqs. (53) imply

\[ e_1(\lambda_\alpha ; \mu)^N = g_2(\lambda_\alpha - \lambda_0 ; \mu) \prod_{\beta=1, \beta \neq \alpha}^{M_1^+} e_2(\lambda_\alpha - \lambda_\beta ; \mu), \]

\[ \alpha = 1, \cdots, M_1^+, \tag{87} \]

\[ g_1(\lambda_0 ; \mu)^N = \prod_{\beta=1}^{M_1^+} g_2(\lambda_0 - \lambda_\beta ; \mu), \tag{88} \]

where

\[ g_n(\lambda ; \mu) = e_n(\lambda \pm \frac{i\pi}{2\mu}; \mu) = \frac{\cosh \mu \left( \lambda + \frac{n\pi}{2} \right)}{\cosh \mu \left( \lambda - \frac{n\pi}{2} \right)}, \tag{89} \]

and \( M = M_1^+ + 1 \). The counting function is now given by

\[ h(\lambda) = \frac{1}{2\pi} \left\{ Nq_1(\lambda ; \mu) - r_2(\lambda - \lambda_0 ; \mu) - \sum_{\beta=1}^{M_1^+} q_2(\lambda - \lambda_\beta ; \mu) \right\}, \tag{90} \]

where \( r_n(\lambda ; \mu) \) is an odd function of \( \lambda \) defined by

\[ r_n(\lambda ; \mu) = i \log g_n(\lambda ; \mu). \tag{91} \]
Proceeding as before, we obtain the density

$$\sigma(b)(\lambda) = s(\lambda) + \frac{1}{N} \left[ \sum_{\alpha=1}^{2} J(\lambda - \tilde{\lambda}_\alpha) - b_1(\lambda - \lambda_0 ; \mu') \right], \quad (92)$$

where

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

$$\hat{b}_n(\omega ; \mu) = -\frac{\sinh\left(\frac{n\omega}{2}\right)}{\sinh\left(\frac{\pi \omega}{\mu}\right)} , \quad 0 < n < \frac{\pi}{\mu}, \quad (93)$$

and $\mu'$ is given by Eq. (82). We determine the center of the negative-parity 1-string, $\lambda_0$, from Eq. (88) by the same procedure used in case (a), and we obtain the same result (84).

Let us examine the quantum numbers of this state:

- We verify by a generalization of the computation (65) that this state also has $S^z = 0$. The energy and momentum are again given by Eq. (75).

- As in case (a), this state is not a parity eigenstate for generic values of $\{\tilde{\lambda}_\alpha\}$. Let us now restrict to the rest frame (85). The Bethe vector is then given by

$$|v\rangle = B\left(\frac{i\pi}{2\mu}\right) \prod_{\alpha=1}^{N-1} B(\lambda_\alpha) \omega_+. \quad (94)$$

Acting with the parity operator using Eq. (84), we obtain

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

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

$$= -(-)^{N/2} |v\rangle. \quad (95)$$

In passing to the second line, we have used the quasi-periodicity property (111), and to arrive at the last line we use the fact that (in the rest frame) the density is an even function of $\lambda$. Thus, the state has parity $-(-)^{N/2}$. The appellation “negative parity” for this string is quite apt!

- Unlike case (a), here the first term of the formula (52) for the charge conjugation eigenvalue does give a contribution, namely, $-1$. (The computation closely parallels the one (86) for case (a).) We conclude that the charge conjugation eigenvalue for this state is also $-(-)^{N/2}$. 

16
We recall that a Boson-antiBoson state with a symmetric (antisymmetric) wavefunction has positive (negative) $\Pi$ and $C$, while for a Fermion-antiFermion state the opposite is true. (See, e.g., Refs. [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]

$$\left(e^{ip(\tilde{\lambda}_1)^N} S(\tilde{\lambda}_1, \tilde{\lambda}_2) - 1 \right) |\tilde{\lambda}_1, \tilde{\lambda}_2\rangle = 0,$$

where $\tilde{\lambda}_1, \tilde{\lambda}_2$ are the hole rapidities, and $p(\lambda)$ is the hole momentum. Combining the definition (59) of the root density with the relation (76) for the hole momentum, we immediately obtain the identity

$$\frac{d}{d\lambda} p(\lambda) + 2\pi \left(\sigma(\lambda) - s(\lambda)\right) = \frac{2\pi}{N} \frac{d}{d\lambda} h(\lambda).$$

Integrating this equation from $-\infty$ to $\tilde{\lambda}_1$, noting that $h(\tilde{\lambda}_1) = \tilde{J}_1$, and then comparing with Eq. (96), we see that the $S$ matrix eigenvalues are given (up to a rapidity-independent phase factor) by

$$S_{(j)} \sim \exp\left\{ i 2\pi N \int_{-\infty}^{\tilde{\lambda}_1} \left(\sigma_{(j)}(\lambda) - s(\lambda)\right) d\lambda \right\}, \quad j = 0, a, b,$$

where $S_{(0)}$, $S_{(a)}$ and $S_{(b)}$ are the eigenvalues of the $S$ matrix corresponding to states (0), (a) and (b), respectively.

Recalling the expression (73) for the density $\sigma_{(0)}(\lambda)$, we obtain

$$S_{(0)} \sim \exp\left\{ i 2\pi \sum_{\alpha=1}^{2} \int_{-\infty}^{\tilde{\lambda}_1} J(\lambda - \tilde{\lambda}_\alpha) \, d\lambda \right\}$$

$$= \exp\left\{ \int_{0}^{\infty} \frac{d\omega}{\omega} \sinh \left(\frac{\pi}{2\mu'} \omega\right) \sinh \left(i\omega\tilde{\lambda}\right) \right\}$$

$$= \prod_{n=0}^{\infty} \frac{\Gamma \left[ \left(1 + \frac{\pi}{\mu'} n - i\tilde{\lambda}\right) / 2 \right] \Gamma \left[ \left(2 + \frac{\pi}{\mu'} n + i\tilde{\lambda}\right) / 2 \right]}{\Gamma \left[ \left(1 + \frac{\pi}{\mu'} n + i\tilde{\lambda}\right) / 2 \right] \Gamma \left[ \left(2 + \frac{\pi}{\mu'} n - i\tilde{\lambda}\right) / 2 \right]}$$

$$\times \frac{\Gamma \left[ \left(\frac{\pi}{\mu'} (n+1) + i\tilde{\lambda}\right) / 2 \right] \Gamma \left[ \left(1 + \frac{\pi}{\mu'} (n+1) - i\tilde{\lambda}\right) / 2 \right]}{\Gamma \left[ \left(\frac{\pi}{\mu'} (n+1) - i\tilde{\lambda}\right) / 2 \right] \Gamma \left[ \left(1 + \frac{\pi}{\mu'} (n+1) + i\tilde{\lambda}\right) / 2 \right]}.$$

(99)
where $\tilde{\lambda} = \tilde{\lambda}_1 - \tilde{\lambda}_2$. Moreover, recalling the expressions (81) and (92) for the densities $\sigma(a)(\lambda)$ and $\sigma(b)(\lambda)$, we obtain

$$\frac{S(a)}{S(0)} = \exp \left\{ -i2\pi \int_{-\infty}^{\tilde{\lambda}_1} a_1(\lambda - \lambda_0 ; \mu') \, d\lambda \right\} = e_1(\frac{\tilde{\lambda}}{2} ; \mu') ,$$

$$\frac{S(b)}{S(0)} = \exp \left\{ -i2\pi \int_{-\infty}^{\tilde{\lambda}_1} b_1(\lambda - \lambda_0 ; \mu') \, d\lambda \right\} = g_1(\frac{\tilde{\lambda}}{2} ; \mu') ,$$

(100)

where again we have used (84). We conclude that the $S$ matrix for the critical XXZ chain is given by

$$S(a) = S(0) \frac{\sinh \left( \mu'(\tilde{\lambda} + i)/2 \right)}{\sinh \left( \mu'(\tilde{\lambda} - i)/2 \right)} , \quad S(b) = S(0) \frac{\cosh \left( \mu'(\tilde{\lambda} + i)/2 \right)}{\cosh \left( \mu'(\tilde{\lambda} - i)/2 \right)} ,$$

(101)

where $S(0)$ is given by Eq. (99), and $\mu'$ is given by Eq. (82). This coincides with the $S$ matrix of sine-Gordon/massive Thirring model [15],[20],[21], provided we identify the sine-Gordon coupling constant $\beta^2$ as

$$\beta^2 = 8 \left( \pi - \mu \right) .$$

(102)

This result has been obtained for the XXZ chain previously, although by less direct means, in Refs. [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 the formula (52) for the charge conjugation eigenvalues of the Bethe Ansatz states, and to better understand states in the critical regime with $S^z \neq 0$. It may be worthwhile to investigate discrete symmetries in integrable chains constructed with higher-rank $R$ matrices, [22],[23] such as $A^{(1)}_{N-1}$ with $N > 2$. 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].

### Acknowledgments

We thank F. Essler and V. Korepin for valuable discussions. This work was supported in part by the National Science Foundation under Grant PHY-9870101.
References

[1] H. Bethe, Z. Phys. 71 (1931) 205.

[2] R. Orbach, Phys. Rev. 112 (1958) 309.

[3] C.N. Yang and C.P. Yang, Phys. Rev. 150 (1966) 321; ibid, 327.

[4] M. Takahashi and M. Suzuki, Prog. Theor. Phys. 48 (1972) 2187.

[5] R.J. Baxter, Ann. Phys. 70 (1972) 193; J. Stat. Phys. 8 (1973) 25; Exactly Solved Models in Statistical Mechanics (Academic Press, 1982).

[6] J.D. Johnson, S. Krinsky, and B.M. McCoy, Phys. Rev. A8 (1973) 2526.

[7] L.D. Faddeev and L.A. Takhtajan, Russ. Math. Surv. 34, 11 (1979); J. Sov. Math. 24 (1984) 241.

[8] P.P. Kulish and E.K. Sklyanin, Phys. Lett. 70A (1979) 461; Lecture Notes in Physics, Vol. 151, (Springer, 1982), p. 61.

[9] F. Woynarovich, J. Phys. A15 (1982) 2985.

[10] A.M. Tsvelick and P.B. Wiegmann, Adv. in Phys. 32 (1983) 453.

[11] H.M. Babujian and A.M. Tsvelick, Nucl. Phys. B265 (1986) 24.

[12] A.N. Kirillov and N.Yu. Reshetikhin, J. Phys. A20 (1987) 1565.

[13] H.J. de Vega, Int. J. Mod. Phys. A4 (1989) 2371.

[14] V.E. Korepin, N.M. Bogoliubov, and A.G. Izergin, Quantum Inverse Scattering Method, Correlation Functions and Algebraic Bethe Ansatz (Cambridge University Press, 1993).

[15] V.E. Korepin, Theor. Math. Phys. 41 (1979) 953.

[16] N. Andrei and C. Destri, Nucl. Phys. B231 (1984) 445.

[17] A. Doikou and R.I. Nepomechie, hep-th/9808012.

[18] J.D. Bjorken and S.D. Drell, Relativistic Quantum Fields (McGraw-Hill, 1965).

[19] T.R. Klassen and E. Melzer, Int. J. Mod. Phys. A8 (1993) 4131.

[20] B. Berg, M. Karowski, W.R. Theis, and H.J. Thun, Phys. Rev. D17 (1978) 1172.
[21] A.B. Zamolodchikov and Al.B. Zamolodchikov, Ann. Phys. 120 (1979) 253.

[22] V.V. Bazhanov, Phys. Lett. 159B (1985) 321; Commun. Math. Phys. 113 (1987) 471.

[23] M. Jimbo, Commun. Math. Phys. 102 (1986) 537; Lecture Notes in Physics, Vol. 246, (Springer, 1986), p. 335.

[24] L. Mezincescu and R.I. Nepomechie, unpublished.