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## LETTER TO THE EDITOR

**Simplified calculation of boundary  $S$  matrices**

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**Abstract.** The antiferromagnetic Heisenberg spin chain with  $N$  spins has a sector with  $N =$  odd, in which the number of excitations is odd. In particular, there is a state with a *single* one-particle excitation. We exploit this fact to give a simplified derivation of the boundary  $S$  matrix for the open antiferromagnetic spin- $\frac{1}{2}$  Heisenberg spin chain with diagonal boundary magnetic fields.

**1. Introduction**

The ground state of the antiferromagnetic spin- $\frac{1}{2}$  Heisenberg spin chain

$$H = \frac{1}{4} \sum_{n=1}^N (\boldsymbol{\sigma}_n \cdot \boldsymbol{\sigma}_{n+1} - 1) \quad \boldsymbol{\sigma}_{N+1} \equiv \boldsymbol{\sigma}_1 \quad (1)$$

lies in the ‘even sector’ (i.e.  $N =$  even). Most investigations of the excitations of this model consider only this sector (see, e.g., [1]), in which the number of excitations is necessarily even.

However, as remarked by Faddeev and Takhtajan [2], there is also the ‘odd sector’ (i.e.  $N =$  odd), in which the number of excitations is odd. In particular, there is a state with a *single* one-particle excitation.

In this letter, we exploit this fact to give a simplified derivation of the boundary  $S$  matrix [3] for the open antiferromagnetic spin- $\frac{1}{2}$  Heisenberg spin chain

$$\mathcal{H} = \frac{1}{4} \left\{ \sum_{n=1}^{N-1} \boldsymbol{\sigma}_n \cdot \boldsymbol{\sigma}_{n+1} + \frac{1}{\xi_-} \sigma_1^z + \frac{1}{\xi_+} \sigma_N^z \right\} \quad (2)$$

where the real parameters  $\xi_{\pm} > \frac{1}{2}$  correspond to boundary magnetic fields. Our analysis follows closely the one in [4], which is a generalization of the approach developed by Korepin–Andrei–Destri [6, 7] to calculate bulk two-particle  $S$  matrices. However, in contrast to [4], we assume that  $N$  is odd and consider one-particle states rather than two-particle states. As a warm-up, we first briefly review the counting of excitations in both the even and odd sectors of the closed spin chain.

**2. Closed chain excitations**

In this section, we briefly review the enumeration of excitations of the closed spin chain, with Hamiltonian given by (1). Upon adopting the ‘string hypothesis’, the Bethe ansatz

equations lead to the following equations for the (real) centres  $\lambda_\alpha^n$  of the strings (see, e.g., [1, 5]),

$$h_n(\lambda_\alpha^n) = J_\alpha^n \tag{3}$$

where  $\alpha = 1, \dots, M_n, n = 1, \dots, \infty$ . The so-called counting function  $h_n(\lambda)$  is defined by

$$h_n(\lambda) = \frac{1}{2\pi} \left\{ Nq_n(\lambda) - \sum_{m=1}^{\infty} \sum_{\beta=1}^{M_m} \Xi_{nm}(\lambda - \lambda_\beta^m) \right\} \tag{4}$$

$\Xi_{nm}(\lambda)$  is given by

$$\Xi_{nm}(\lambda) = (1 - \delta_{nm})q_{|n-m|}(\lambda) + 2q_{|n-m|+2}(\lambda) + \dots + 2q_{n+m-2}(\lambda) + q_{n+m}(\lambda) \tag{5}$$

and  $q_n(\lambda)$  is the odd monotonic-increasing function defined by

$$q_n(\lambda) = \pi + i \log \left( \frac{\lambda + \frac{1}{2}in}{\lambda - \frac{1}{2}in} \right) \quad -\pi < q_n(\lambda) \leq \pi. \tag{6}$$

Moreover,  $\{J_\alpha^n\}$  are integers or half-odd integers which satisfy

$$-J_{\max}^n \leq J_\alpha^n \leq J_{\max}^n \tag{7}$$

where  $J_{\max}^n$  is given by

$$J_{\max}^n = \frac{1}{2}(N + M_n - 1) - \sum_{m=1}^{\infty} \min(m, n)M_m. \tag{8}$$

We regard  $\{J_\alpha^n\}$  as ‘quantum numbers’ which parametrize the Bethe ansatz states. For every set  $\{J_\alpha^n\}$  in the range given by (7) (no two of which are identical), we assume that there is a unique solution  $\{\lambda_\alpha^n\}$  (no two of which are identical) of (3).

The energy, momentum, and spin eigenvalues of the Bethe ansatz states are given by

$$E = -\pi \sum_{n=1}^{\infty} \sum_{\alpha=1}^{M_n} a_n(\lambda_\alpha^n) \tag{9}$$

$$P = - \sum_{n=1}^{\infty} \sum_{\alpha=1}^{M_n} [q_n(\lambda_\alpha^n) - \pi] \tag{10}$$

$$S = S^z = \frac{N}{2} - \sum_{n=1}^{\infty} nM_n \tag{11}$$

where

$$a_n(\lambda) = \frac{1}{2\pi} \frac{dq_n(\lambda)}{d\lambda} = \frac{1}{2\pi} \frac{n}{\lambda^2 + (n^2/4)}. \tag{12}$$

The number of holes (excitations)  $\nu$  in a given Bethe ansatz state is given by

$$\begin{aligned} \nu &= \text{number of vacancies for } J_\alpha^1\text{s} - \text{number of } J_\alpha^1\text{s} \\ &= (J_{\max}^1 - J_{\min}^1 + 1) - M_1. \end{aligned} \tag{13}$$

The ground state lies in the even sector, with  $M_1 = (N/2)$ , and  $M_n = 0$  for  $n > 1$ . We see from (8) that this state has  $J_{\max}^1 = (N/4) - \frac{1}{2}$ . Therefore, the ground state has no holes; i.e. it is a ‘filled Fermi sea’, with (see (11)) spin  $S = S^z = 0$ . Further calculations show that, for  $N \rightarrow \infty$ , the energy and momentum of the ground state are given by

$$E_0 = -N \log 2 \quad P_0 = \frac{N\pi}{2}. \tag{14}$$

Consider now the state in the odd sector with  $M_1 = (N/2) - \frac{1}{2}$  and  $M_n = 0$  for  $n > 1$ . This state has  $J_{\max}^1 = (N/4) - \frac{1}{4}$ , and therefore it has one hole. This state has spin  $S = S^z = \frac{1}{2}$ . Moreover, calculations along the lines of [1, 5] show that the energy and momentum are given by

$$E = E_0 + \varepsilon(\tilde{\lambda}) \quad P = P_0 + p(\tilde{\lambda}) \quad (15)$$

where  $E_0$  and  $P_0$  are given by (14),

$$\varepsilon(\lambda) = \frac{\pi}{2 \cosh \pi \lambda} \quad p(\lambda) = \tan^{-1}(\sinh \pi \lambda) - \frac{\pi}{2} \quad (16)$$

and  $\tilde{\lambda}$  corresponds to the hole rapidity. This state consists of a single particle-like excitation ('kink' or 'spinon') with spin- $\frac{1}{2}$ , energy  $\varepsilon(\tilde{\lambda})$  and momentum  $p(\tilde{\lambda})$ . The energy-momentum dispersion relation is

$$\varepsilon = -\frac{\pi}{2} \sin p. \quad (17)$$

Similarly, one can show that there exist states with any (non-negative) integer number  $\nu$  of excitations with the above dispersion relation. States with  $\nu = \text{even}$  lie in the even sector, while states with  $\nu = \text{odd}$  lie in the odd sector. The total energy and momentum are given by

$$E = E_0 + \sum_{\alpha=1}^{\nu} \varepsilon(\tilde{\lambda}_{\alpha}) \quad P = P_0 + \sum_{\alpha=1}^{\nu} p(\tilde{\lambda}_{\alpha}). \quad (18)$$

Note that  $E_0$  and  $P_0$  (which are given by (14)) correspond to the ground-state energy and momentum only for  $N = \text{even}$ . Indeed, for  $N \rightarrow \infty$ , the energy of a state with any finite number of excitations has an infinite contribution  $E_0$  which must be subtracted. In order to interpret the remaining finite part as the energy of the excitations, different subtractions must be performed in the even and odd sectors of the model.

### 3. Open chain excitations

We turn now to the open spin chain, with Hamiltonian  $\mathcal{H}$  given by (2). The simultaneous eigenstates of  $\mathcal{H}$  and  $S^z$  have been determined by both the coordinate [8, 9] and algebraic [10] Bethe ansatz.

Using the string hypothesis, the Bethe ansatz equations become [4]

$$h_n(\lambda_{\alpha}^n) = J_{\alpha}^n \quad (19)$$

where the counting function  $h_n(\lambda)$  is now given by

$$h_n(\lambda) = \frac{1}{2\pi} \left\{ (2N+1)q_n(\lambda) + \sum_{l=1}^n [q_{n+2\xi_+-2l}(\lambda) + q_{n+2\xi_--2l}(\lambda)] \right. \\ \left. - \sum_{m=1}^{\infty} \sum_{\beta=1}^{M_m} [\Xi_{nm}(\lambda - \lambda_{\beta}^m) + \Xi_{nm}(\lambda + \lambda_{\beta}^m)] \right\}. \quad (20)$$

The requirement that Bethe ansatz solutions correspond to independent Bethe ansatz states leads to the restriction  $\lambda_{\alpha}^n > 0$ . The 'quantum numbers'  $\{J_{\alpha}^n\}$  are integers in the range

$$J_{\min}^n \leq J_{\alpha}^n \leq J_{\max}^n \quad (21)$$

where

$$J_{\max}^n - J_{\min}^n = N + M_n - 2 \left( \sum_{m=1}^{\infty} \min(m, n) M_m \right) - 1. \quad (22)$$

For simplicity, we assume that  $2\xi_{\pm}$  is not an integer, and  $\xi_{\pm} > \frac{1}{2}$ .

The expressions for the energy and  $S^z$  eigenvalues are the same as for the closed chain, namely (9) and (11), respectively. (Of course, momentum and total spin are not good quantum numbers for the open chain.)

As in the case of the closed chain, the Bethe ansatz state with a single one-particle excitation lies in the odd sector with  $M_1 = (N/2) - \frac{1}{2}$  and  $M_n = 0$  for  $n > 1$ . (The number of holes is again given by (13).) This state has  $S^z = \frac{1}{2}$ .

We shall need in the next section the density  $\sigma(\lambda)$  of roots and hole for this state, which is defined by

$$\sigma(\lambda) = \frac{1}{N} \frac{dh_1(\lambda)}{d\lambda}. \quad (23)$$

Passing with care from the sum in  $h_1(\lambda)$  to an integral, we obtain an integral equation, whose solution is given by

$$\sigma(\lambda) = 2s(\lambda) + \frac{1}{N} r^{(+)}(\lambda) \quad (24)$$

where

$$r^{(+)}(\lambda) = s(\lambda) + J(\lambda) + J_+(\lambda) + J_-(\lambda) + J(\lambda - \tilde{\lambda}) + J(\lambda + \tilde{\lambda}) \quad (25)$$

(plus terms that are higher order in  $1/N$ ),  $\tilde{\lambda}$  is the hole rapidity, and

$$\begin{aligned} s(\lambda) &= \frac{1}{2 \cosh \pi \lambda} = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega\lambda} \frac{e^{-|\omega|/2}}{1 + e^{-|\omega|}} \\ J(\lambda) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega\lambda} \frac{e^{-|\omega|}}{1 + e^{-|\omega|}} \\ J_{\pm}(\lambda) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega\lambda} \frac{e^{-(\xi_{\pm} - \frac{1}{2})|\omega|}}{1 + e^{-|\omega|}}. \end{aligned} \quad (26)$$

#### 4. Boundary $S$ matrix

The boundary  $S$  matrix describes the interaction of an excitation with the ends of the spin chain. The  $U(1)$  symmetry of the Hamiltonian boundary terms implies that the boundary  $S$  matrix is of the diagonal form

$$\mathcal{K}(\lambda, \xi) = \begin{pmatrix} \alpha(\lambda, \xi) & 0 \\ 0 & \beta(\lambda, \xi) \end{pmatrix}. \quad (27)$$

We therefore need to explicitly determine the matrix elements  $\alpha(\lambda, \xi)$  and  $\beta(\lambda, \xi)$ , which are the boundary scattering amplitudes for excitations with  $S^z = +\frac{1}{2}$  and  $S^z = -\frac{1}{2}$ , respectively.

We proceed by examining states  $|\tilde{\lambda}\rangle_a$  with a single one-particle excitation of rapidity  $\tilde{\lambda}$ . The isotopic index  $a$  is suppressed below. For such states, the following simple quantization condition holds:

$$(e^{i2p(\tilde{\lambda})N} \mathcal{K}(\tilde{\lambda}, \xi_-) \mathcal{K}(\tilde{\lambda}, \xi_+) - 1) |\tilde{\lambda}\rangle = 0. \quad (28)$$

Here  $p(\tilde{\lambda})$  is defined by (16), which is the expression for the momentum of a particle with rapidity  $\tilde{\lambda}$  for the corresponding system with periodic boundary conditions.

For the  $S^z = +\frac{1}{2}$  state, the quantization condition implies

$$2p(\tilde{\lambda}) + \frac{1}{N} \Phi^{(+)} = \frac{2\pi}{N} m \quad (29)$$

where  $m$  is an integer and

$$e^{i\Phi^{(+)}} = \alpha(\tilde{\lambda}, \xi_-) \alpha(\tilde{\lambda}, \xi_+). \quad (30)$$

On the other hand, one can derive the identity [4, 5]

$$2p(\tilde{\lambda}) + \frac{2\pi}{N} \int_0^{\tilde{\lambda}} r^{(+)}(\lambda) d\lambda + \text{constant} = \frac{2\pi}{N} \tilde{J} \quad (31)$$

where  $r^{(+)}(\lambda)$  is the quantity introduced in (24). Comparing this result with (29), it follows that

$$\Phi^{(+)} = 2\pi \int_0^{\tilde{\lambda}} r^{(+)}(\lambda) d\lambda + \text{constant}. \quad (32)$$

Using the explicit expressions given in (25) and (26) for  $r^{(+)}(\lambda)$ , we obtain the following result for  $\alpha(\lambda, \xi)$  (up to a rapidity-independent phase factor):

$$\alpha(\lambda, \xi) = \frac{\Gamma(-\frac{1}{2}i\lambda + \frac{1}{4})}{\Gamma(\frac{1}{2}i\lambda + \frac{1}{4})} \frac{\Gamma(\frac{1}{2}i\lambda + 1)}{\Gamma(-\frac{1}{2}i\lambda + 1)} \frac{\Gamma(-\frac{1}{2}i\lambda + \frac{1}{4}(2\xi - 1))}{\Gamma(\frac{1}{2}i\lambda + \frac{1}{4}(2\xi - 1))} \frac{\Gamma(\frac{1}{2}i\lambda + \frac{1}{4}(2\xi + 1))}{\Gamma(-\frac{1}{2}i\lambda + \frac{1}{4}(2\xi + 1))}. \quad (33)$$

To determine the remaining element  $\beta(\lambda, \xi)$  of the boundary  $S$  matrix, we consider the  $S^z = -\frac{1}{2}$  state. The quantization condition implies

$$2p(\tilde{\lambda}) + \frac{1}{N} \Phi^{(-)} = \frac{2\pi}{N} m \quad (34)$$

with

$$e^{i\Phi^{(-)}} = \beta(\tilde{\lambda}, \xi_-) \beta(\tilde{\lambda}, \xi_+). \quad (35)$$

The  $S^z = -\frac{1}{2}$  state is most easily described within the Bethe ansatz approach by changing the pseudovacuum to the state with all spins down. Sklyanin has shown [10] that there is a corresponding change  $\xi_{\pm} \rightarrow -\xi_{\pm}$  in the Bethe ansatz equations. The expression for the energy eigenvalues remains the same, but the expression for the  $S^z$  eigenvalues becomes

$$S^z = \sum_{n=1}^{\infty} n M_n - \frac{N}{2}. \quad (36)$$

The  $S^z = -\frac{1}{2}$  state now corresponds to the Bethe ansatz state consisting of one hole in the Fermi sea ( $M_1 = (N/2) - \frac{1}{2}$  and  $M_n = 0$  for  $n > 1$ ). The calculation of the corresponding function  $r^{(-)}(\lambda)$  is exactly the same as for  $r^{(+)}(\lambda)$ , except that we must track the change  $\xi_{\pm} \rightarrow -\xi_{\pm}$ . We find that  $\beta(\lambda, \xi)$  is given (up to a multiplicative constant) by

$$\beta(\lambda, \xi) = -\frac{\lambda + i(\xi - \frac{1}{2})}{\lambda - i(\xi - \frac{1}{2})} \alpha(\lambda, \xi) \quad (37)$$

where  $\alpha(\lambda, \xi)$  is given by (33). This completes the derivation of the boundary  $S$  matrix.

**5. Discussion**

We have seen that, by considering one-particle states, the boundary  $S$  matrix for the open Heisenberg chain can be obtained in a most direct and straightforward manner. We expect that this approach can be used quite generally to calculate boundary  $S$  matrices for integrable models with boundaries whose Bethe ansatz equations are known and, in particular, for the models for which the method of [4] has already been successfully applied (see, e.g., [11–13]). We are now using this approach to compute [14] the boundary  $S$  matrix for the anisotropic spin- $\frac{1}{2}$  chain, which was first calculated using the vertex operator method [15].

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