

## **Bethe Ansatz for an Open Heisenberg Spin Chain with Impurity**

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*Received February 8, 1993*

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We have set up the algebraic Bethe ansatz equation for an open Heisenberg spin chain having an impurity of a different type of spin. The chain is considered to be open and hence the QISM approach as modified by Sklyanin is used to set up the equations for the Bethe ansatz.

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### **1. INTRODUCTION**

One of the earliest integrable nonlinear systems is the Heisenberg spin chain, initially studied by Onsager (1944). Later Yang (1967), Bethe (1931), Baxter (1972), Sutherland (1968), and many other physicists turned their attention to the study of the model itself and its various generalizations. Later, after the invention of the quantum inverse scattering method (QISM) (Faddeev, 1980), it became clear that there exists a close relation between the original coordinate-dependent Bethe ansatz, the partition function technique and statistical mechanics, and the approach of QISM. The powerful methodology of QISM made it possible to introduce boundary conditions other than the periodic one and the first such concrete formulation was put forward by Sklyanin (1988). On the other hand, from the practical standpoint, it is quite justified to assume that the spin chain may contain not only one type of atom of definite spin, but also some kind of impurity having a different spin (some atom with spin value not equal to  $1/2$ ). In this communication we study an open Heisenberg spin chain of spin  $1/2$  containing an impurity of spin  $S$ . Since it is contained in a finite open region the periodic boundary condition is not applicable.

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## 2. FORMULATION

The Heisenberg chain is a linear lattice of spin-1/2 objects  $\sigma_k$ , with  $k$  being the lattice position and the  $\sigma$  Pauli matrix. We allow the system to interact with an isolated impurity at the  $m$ th lattice site. The Hamiltonians corresponding to the pure spin chain and the interaction with the impurity are

$$H_0 = \frac{1}{2} J \sum \sigma_k \cdot \sigma_{k+1} \quad (1)$$

$$H_I = \frac{2J}{(2s+1)^2} \left\{ \sigma_m \cdot \mathbf{s} + \sigma_{m+1} \cdot \mathbf{s} + \frac{1}{2} \times [\sigma_m \cdot \mathbf{s}, \sigma_{m+1} \cdot \mathbf{s} - s(s+1)\sigma_m \cdot \sigma_{m+1}] \right\} \quad (2)$$

It has been observed that it is more convenient to start with the transfer matrix rather than the Hamiltonian. The construction of the transfer matrix is standard and rests on the consideration of the local vertices.

In our case the local vertex can be written as

$$L_{0j}^s(\lambda) = \frac{\lambda + 1/2 + \sigma_0 \otimes \sigma_j}{i\lambda + s + 1/2} \quad (3)$$

which acts in the tensor product of the auxiliary space  $V_0$  (space of spin 1/2) and the space  $V_j$  (carrying the spin representation at the  $j$ th site);  $\lambda$  is a complex parameter. On the other hand the pure spin-1/2 vertex is written as

$$L_{0j}^{1/2}(\lambda) = \frac{\lambda + 1/2 + (1/2)\sigma_0 \otimes \sigma_j}{\lambda + 1} \quad (4)$$

The transfer matrix is found to be

$$T(\lambda) = \text{Tr}_0 \{ L_{0N}^{1/2}(\lambda) L_{0N-1}^{1/2}(\lambda) \cdots L_{0m+1}^{1/2}(\lambda) L_{0m}^s(\lambda) \cdots L_{01}^{1/2}(\lambda) \} = \text{Tr}_0 \tau$$

$\tau$  is the monodromy matrix. Both the vertices given in equations (3) and (4) are intertwined by the same quantum  $R$ -matrix, due to the relations

$$\begin{aligned} R(\lambda, \mu) [L_{0j}^{1/2}(\lambda) \otimes 1] [1 \otimes L_{0j}^{1/2}(\mu)] \\ = [1 \otimes L_{0j}^{1/2}(\mu) (L_{0j}^{1/2}(\lambda) \otimes 1)] R(\lambda, \mu) \end{aligned} \quad (5)$$

and

$$\begin{aligned} R(\lambda, \mu) [L_{0m}^s(\lambda) \otimes 1] [1 \otimes L_{0m}^s(\mu)] \\ = [1 \otimes L_{0m}^s(\mu) [L_{0m}^s(\lambda) \otimes 1]] R(\lambda, \mu) \end{aligned} \quad (6)$$

where the  $R$  matrix is explicitly written as

$$R(\lambda, \mu) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & (\lambda - \mu)/(\lambda - \mu + \eta) & \eta/(\lambda - \mu + \eta) & 0 \\ 0 & \eta/(\lambda - \mu + \eta) & (\lambda - \mu)/(\lambda - \mu + \eta) & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \quad (7)$$

It is now easy to prove that the matrix  $T(\lambda)$  also satisfies

$$R(\lambda, \mu)[T(\lambda) \otimes 1][1 \otimes T(\mu)] = [1 \otimes T(\mu)][T(\lambda) \otimes 1]R(\lambda, \mu) \quad (8)$$

which actually is the basis for the application of the QISM technique. On the other hand, recently an extension of this methodology was suggested by Sklyanin (1988), which takes into account boundary conditions other than the periodic one—a situation which is realized in an open spin chain. Another important feature of this modified approach is that now we can analyze the system on a finite portion of the axis. In this formalism the boundary conditions are introduced by two matrices  $K^+$  and  $K^-$  which obey the following two equations (Dasgupta and Roy Chowdhury, 1992):

$$\begin{aligned} &R(\lambda, \mu)K_-(\mu)R(\lambda + \mu - \eta)K_-^2(\mu) \\ &= K_-^2(\mu)R(\lambda + \mu - \eta)K_-(\lambda)R(\lambda - \mu) \\ &R(-\lambda + \mu)K_+^{1t_1}(\lambda)R(-\lambda - \mu - \eta)K_+^{2t_2}(\mu) \\ &= K_+^{2t_2}(\mu)R(-\lambda - \mu - \eta)K_+^{1t_1}(\lambda)R(-\lambda + \mu) \end{aligned} \quad (9)$$

In our present situation we have

$$\begin{aligned} K_+ &= \begin{bmatrix} 2\lambda + \eta - \xi_+ & 0 \\ 0 & -(2\lambda + \eta + \xi_+) \end{bmatrix} \\ K_- &= \begin{bmatrix} 2\lambda - \eta - \xi_- & 0 \\ 0 & -(2\lambda - \eta + \xi_-) \end{bmatrix} \end{aligned}$$

Then the modified transfer matrix can be written as

$$t(u) = \text{tr}[K_+(\lambda)u(\lambda)] \quad (10)$$

where

$$\begin{aligned} u(\lambda) &= T(\lambda)K_-(\lambda)\sigma_2 T(-\lambda)\sigma_2 \\ &= \begin{bmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{bmatrix} \end{aligned} \quad (11)$$

where  $T(\lambda)$  stands for the monodromy matrix for the usual case with closed end. It can then be demonstrated that  $u(\lambda)$  also satisfies

$$\begin{aligned} &R(\lambda_{12})u^1(\lambda_1)R(\bar{\lambda}_{12} + \eta)u^2(\lambda_2) \\ &= u^2(\lambda_2)R(\bar{\lambda}_{12} - \eta)u^1(\lambda_1)R(\lambda_{12}) \end{aligned}$$

where

$$\begin{aligned} u^1(\lambda) &= u(\lambda) \otimes 1, & u^2(\lambda) &= 1 \otimes u(\lambda) \\ \lambda_{12} &= \lambda_1 - \lambda_2, & \bar{\lambda}_{12} &= \lambda_1 + \lambda_2 \\ \lambda_{0i} &= \lambda - \lambda_i, & \bar{\lambda}_0 &= \lambda + \lambda_i \end{aligned} \quad (12)$$

With the explicit form of  $u$  given in (1), we can use (12) to set up the commutation rules required to set up the algebraic Bethe ansatz:

$$\begin{aligned} A(\lambda)B(\mu) &= \frac{a(\mu - \lambda)b(\lambda + \mu + \eta)}{a(\lambda + \mu - \eta)b(\mu - \lambda)} B(\mu)A(\lambda) \\ &\quad - \frac{b(\lambda + \mu - \eta)C(\mu - \lambda)}{a(\lambda + \mu - \eta)b(\mu - \lambda)} B(\lambda)A(\mu) \\ &\quad - \frac{C(\lambda + \mu - \eta)}{a(\lambda + \mu - \eta)} B(\lambda)D(\mu) \\ D(\lambda)B(\mu) &= \frac{C(\lambda + \mu - \eta)}{a(\lambda + \mu - \eta)b(\lambda - \mu)} \left[ \frac{a^2(\lambda - \mu)}{b(\lambda - \mu)} + \frac{C(\lambda - \mu)c(\mu - \lambda)}{b(\mu - \lambda)} \right] \\ &\quad \times B(\lambda)A(\mu) + \frac{C(\lambda + \mu - \eta)C(\lambda - \mu)}{a(\lambda + \mu - \eta)b(\lambda - \mu)} \left[ \frac{a(\lambda - \mu)}{b(\lambda - \mu)} + \frac{(\mu - \lambda)}{b(\mu - \lambda)} \right] \\ &\quad \times B(\mu)A(\lambda) + \frac{c(\lambda - \mu)}{a(\lambda + \mu - \eta)} \frac{C^2(\lambda + \mu - \eta) - a^2(\lambda + \mu - \eta)}{b(\lambda - \mu)b(\lambda + \mu - \eta)} \\ &\quad \times B(\lambda)D(\mu) + \frac{a(\lambda - \mu)}{b(\lambda - \mu)} \frac{a^2(\lambda + \mu - \eta) - c^2(\lambda + \mu - \eta)}{a(\lambda + \mu - \eta)b(\lambda + \mu - \eta)} \\ &\quad \times B(\mu)D(\lambda) \end{aligned} \quad (13)$$

The other commutation rules implied by equation (2) are not written here, as we will not require them.

### 3. CONSTRUCTION OF BETHE STATES

The construction of the Bethe states starts with the observation that the Hamiltonian can be written as

$$\begin{aligned} t(\lambda) &= \text{Tr}[K_+(\lambda)u(\lambda)] \\ &= \frac{(2\lambda + \eta)(2\lambda - \eta - \xi_+)}{2\lambda} A(\lambda) - \frac{2\lambda + n + \xi_+}{2\lambda} \tilde{D}(\lambda) \\ &= \alpha A(\lambda) - B\tilde{D}(\lambda) \quad (\text{say}) \end{aligned} \quad (14)$$

where we have defined

$$\tilde{u}(\lambda) = \begin{bmatrix} \tilde{D}(\lambda) & -\tilde{B}(\lambda) \\ -\tilde{C}(\lambda) & \tilde{A}(\lambda) \end{bmatrix} \tag{15}$$

the algebraic adjunct of  $u(\lambda)$ , via

$$\begin{aligned} \tilde{u}(\lambda) &= 2 \operatorname{tr}_2 P_{12}^{-1} u(\lambda) R_{12}(2\lambda) \\ &= \begin{bmatrix} -C(2\lambda)A(\lambda) + b(2\lambda)D(\lambda) & -a(2\lambda)B(\lambda) \\ -a(2\lambda)C(\lambda) & b(2\lambda)A(\lambda) - C(2\lambda)D(\lambda) \end{bmatrix} \end{aligned} \tag{16}$$

The main purpose of defining the new monodromy matrix  $\tilde{u}$  is that in these new variables the commutation rules (13) can be reduced to a simpler form

$$\begin{aligned} A(\lambda)B(\lambda) &= \frac{(\lambda - \mu - \eta)(\lambda + \mu - \eta)}{(\lambda + \mu)(\lambda - \mu)} B(\mu)A(\lambda) + \frac{\eta(2\mu - \eta)}{2\mu(\lambda - \mu)} B(\lambda)A(\mu) \\ &\quad - \frac{\eta}{2\mu(\lambda + \mu)} B(\lambda)\tilde{D}(\mu) \\ \tilde{D}(\lambda)B(\mu) &= \frac{\eta(2\lambda + \eta)(2\mu - \eta)}{2\mu(\lambda + \mu)} B(\lambda)A(\mu) - \frac{\eta(2\lambda + \eta)}{2\mu(\lambda - \mu)} B(\lambda)\tilde{D}(\mu) \\ &\quad + \frac{(\lambda - \mu + \eta)(\lambda + \mu + \eta)}{(\lambda + \mu)(\lambda - \mu)} B(\mu)\tilde{D}(\lambda) \end{aligned} \tag{17}$$

We now assume the existence of a vacuum state, which in the present case can be represented as

$$|0\rangle = |e_1^{1/2}\rangle \otimes \cdots \otimes |e_m^{1/2}\rangle \otimes |e_{m,s}^s\rangle \otimes \cdots \otimes |e_N^{1/2}\rangle \tag{18}$$

where  $|e_i^{1/2}\rangle$  is the vacuum vector corresponding to spin 1/2 and  $|e_{m,s}^s\rangle$  is the same for the spin- $s$  impurity. With this structure of the lowest state  $|0\rangle$  we easily observe that

$$\begin{aligned} A(\lambda)|0\rangle &= (i\lambda + 1)^N (i\lambda + 1/2 + s)|0\rangle \\ D(\lambda)|0\rangle &= (i\lambda)^N (i\lambda + 1/2 - s)|0\rangle \\ C(\lambda)|0\rangle &= 0 \end{aligned} \tag{19}$$

and the  $M$ -particle excitation is constructed by  $B(\lambda_i)$

$$|\Psi(\lambda_1 \cdots \lambda)\rangle = \prod_{i=1}^M B(\lambda_i)|0\rangle \tag{20}$$

From the definition of  $\tilde{u}(\lambda)$  we can at once deduce

$$\begin{aligned} \tilde{D}(\lambda)|0\rangle &= (2\lambda - \eta)(2\lambda + n + \xi_-)(-i\lambda + 1)^N(-1\lambda + 1/2 + s) \\ &\quad \times (-i\lambda)^N(i\lambda + 1/2 - s)|0\rangle \\ A(\lambda)|0\rangle &= -(2\lambda - \eta - \xi_-)(i\lambda + 1)^N(i\lambda + 1/2 + s)(-i\lambda)^N \\ &\quad \times (-i\lambda + 1/2 - s)|0\rangle \end{aligned} \tag{21}$$

Now operating with  $t(\lambda)$  given in equation (14) on  $|\Psi(\lambda_1 \dots \lambda_M)\rangle$  and using the commutation rules (17) to evaluate the unwanted terms, we get

$$\begin{aligned} &\frac{(2\lambda_i + \eta + \xi_-)(-i\lambda_i + 1)^M(-i\lambda_i + 1/2 + s)(i\lambda_i)^M(i\lambda_i + 1/2 - s)}{(2\lambda_i - \eta - \xi_-)(i\lambda_i + 1)^M(i\lambda_i + 1/2 + s)(-i\lambda_i)^M(-i\lambda_i + 1/2 - s)} \\ &= \frac{(2\lambda_i - n - \xi_+)}{(2\lambda_i + n + \xi_+)} \prod_{\substack{j=1 \\ j \neq i}}^M \frac{(\lambda_{ij} - \eta)(\bar{\lambda}_{ij} - \eta)}{(\lambda_{ij} + \eta)(\bar{\lambda}_{ij} + \eta)} \end{aligned} \tag{22}$$

This is the coupled set of equations for the momenta  $\lambda_i$  ( $i = 1, \dots, M$ ). The eigenvalue of the corresponding state  $|\Psi(\lambda_1 \dots \lambda_M)\rangle$  is given as

$$\begin{aligned} E_M &= \frac{1}{D} \left( 1 + \frac{n}{2\lambda_0} \right) \left[ (2\lambda_0 - n - \xi_+) \prod_{\substack{i=1 \\ i \neq j}}^n (\lambda_{0i} - \eta)(\bar{\lambda}_{0i} - \eta) \right] \\ &\quad \times (i\lambda_0 + 1)^M \left( i\lambda_0 + \frac{1}{2} + s \right) - \frac{1}{2\lambda_0 D} \left[ (2\lambda_0 + n + \xi_+) \right. \\ &\quad \left. \times \prod_{\substack{i=1 \\ j \neq i}}^M (\lambda_{0i} + \eta)(\bar{\lambda}_{0i} + \eta) \right] (i\lambda_0)^N \left( i\lambda_0 + \frac{1}{2} - s \right) \end{aligned} \tag{23}$$

with

$$D = \prod_{i=1}^N \lambda_{0i} \bar{\lambda}_{0i}$$

### 4. INTEGRAL EQUATION

From the form of equation (22) it is quite clear that it is impossible to solve it explicitly. What is usually done is to convert (22) into an integral equation for the density of the eigenvalues  $\lambda_i$  in the interval  $(\lambda_i, \lambda_i + d\lambda_i)$  as  $M \rightarrow \infty$ . For this we take the logarithm of both sides of (22) and obtain

$$\begin{aligned} N \ln \left( \frac{1 - i\lambda_i}{1 + i\lambda_i} \right) &= \ln \left[ \frac{(s + 1/2 + i\lambda_i)(-s + 1/2 - i\lambda_i)}{(-i\lambda_i + 1/2 + s)(i\lambda_i + 1/2 - s)} \right] \\ &\quad + \ln \left[ \frac{(2\lambda_i - \eta - \xi_+)(2\lambda_i - \eta - \xi_-)}{(2\lambda_i + \eta + \xi_+)(2\lambda_i + \eta + \xi_-)} \right] \\ &\quad + \sum_{\substack{i=1 \\ i \neq j}}^M \ln \frac{\lambda_{ij} - \eta}{\lambda_{ij} + \eta} + \sum_{\substack{i=1 \\ i \neq j}}^M \ln \left( \frac{\bar{\lambda}_{ij} - \eta}{\lambda_{ij} + \eta} \right) \end{aligned} \tag{24}$$

Let us now set

$$\phi(\lambda_i) = \frac{1}{N} \left[ \Psi(\lambda_i) + \chi(\lambda_i) + \sum_j \{ \theta(\lambda_{ij}) + \theta(\bar{\lambda}_{ij}) \} \right] + \frac{2\pi n_i}{N}$$

where the functions  $\phi$ ,  $\Psi$ ,  $\chi$ , and  $\theta$  are defined as follows:

$$\begin{aligned} \phi(\lambda_i) &= \ln \left( \frac{1 - i\lambda_i}{1 + i\lambda_i} \right) \\ \Psi(\lambda_i) &= \ln \left[ \frac{(i\lambda_i + 1/2 + s)(-i\lambda_i + 1/2 - s)}{(-i\lambda_i + 1/2 + s)(i\lambda_i + 1/2 - s)} \right] \\ \chi(\lambda_i) &= \ln \left[ \frac{(2\lambda_i - \eta - \xi_+)(2\lambda_i - \eta - \xi_-)}{(2\lambda_i + \eta + \xi_+)(2\lambda_i + \eta + \xi_-)} \right] \\ \theta(\lambda_i) &= \ln \left[ \frac{\lambda_{ij} - \eta}{\lambda_{ij} + \eta} \right] \end{aligned} \tag{25}$$

Changing  $i$  to  $i + 1$  in equation (24) and subtracting (24) from the new equation we get (after proceeding to the limit  $N \rightarrow \infty$ )

$$\frac{d\Phi(\lambda)}{d\lambda} = + \int_{-\lambda}^{\lambda} \rho(\lambda') K(\lambda - \lambda') d\lambda' + \rho(\lambda) g(\lambda)$$

where the kernel  $K$  is given by

$$K = \frac{d}{dx} [\theta(x - x') + \theta(x + x')]$$

and  $g$  is defined by

$$g = 2\pi + \frac{d\Psi}{dx} + \frac{d\chi}{dx}$$

### 5. DISCUSSION

In our above analysis we have constructed the algebraic Bethe ansatz for a Heisenberg spin chain with impurity of a different spin but without the usual periodic boundary condition. The integral equation derived for the density of the eigenvalues is of Fredholm type and as such can be solved by usual methods.

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