

# Boundary energy of the quantum spin chain with various boundary terms

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Quantum integrable systems have many applications in

- String/ Gauge theories: AdS/CFT, Super-symmetric Yang-Mills theories...
- Statistical mechanics: The Ising model, the six-vertex models...
- Condensed Matter Physics: The super-symmetric  $t - J$  Model, the Hubbard model...
- Mathematics: Quantum group, Representation theory, Algebraic Topology, ...

# I. Introduction

Methods to solve the spectrum

There are many methods to solve quantum integrable systems (The case of  $T = 0$ ):

- The Coordinate Bethe Ansatz method (Bethe 1931)
- The Baxter's  $T - Q$  relation method (Baxter 1970s )
- The Quantum Inverse Scattering (or Algebraic Bethe Ansatz) method (Faddeev's School 1979s) and its generalizations (such as the analytic Bethe Ansatz method (Reshetikhin 1983 and Mezincescu & Nepomechie 1992, the separation of variables method (Sklyanin 1985, the Lyon's group 2013), the q-Onsager algebra approach (Baseilhac 2006))
- The off-diagonal Bethe Ansatz method (Wang's school 2013s)
- The modified algebraic Bethe Ansatz (Belliard et. al 2013s)

⋮

## II. Heisenberg Chains: With $U(1)$ -symmetry

Periodic boundary condition

The Hamiltonian of the closed Heisenberg chain is

$$H = \sum_{k=1}^N \left( \sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y + \sigma_k^z \sigma_{k+1}^z \right),$$

where

$$\sigma_{N+1}^\alpha = \sigma_1^\alpha, \quad \alpha = x, y, z.$$

The system is **integrable**, i.e., there exist enough conserved charges

$$i\hbar \frac{\partial}{\partial t} h_i = [H, h_i] = 0, \quad i = 1, \dots$$

and

$$[h_i, h_j] = 0.$$

## II. Heisenberg Chains: With $U(1)$ -symmetry

Periodic boundary condition

It is convenient to introduce a generation function of these charges, the so-called transfer matrix

$$t(u) = \sum_{i=0} h_i u^i.$$

Then

$$[t(u), t(v)] = 0, \quad H \propto \frac{\partial}{\partial u} \ln t(u)|_{u=0} + \text{const},$$

or

$$H \propto h_0^{-1} h_1 + \text{const},$$

$$h_0 \sigma_i^\alpha h_0^{-1} = \sigma_{i+1}^\alpha.$$

## II. Heisenberg Chains: With $U(1)$ -symmetry

Periodic boundary condition

The eigenstates and the corresponding eigenvalues can be obtained by Quantum Inverse Scattering Method (QISM). In the framework of QISM, the monodromy matrix  $T(u)$

$$T(u) = \begin{pmatrix} A(u) & B(u) \\ C(u) & D(u) \end{pmatrix},$$

has played a central role. It is built from the six-vertex R-matrix of

$$T_0(u) = R_{0N}(u - \theta_N) \dots R_{01}(u - \theta_1),$$

where the well-known six-vertex R-matrix is given by

$$R(u) = \begin{pmatrix} u + \eta & & & \\ & u & \eta & \\ & \eta & u & \\ & & & u + \eta \end{pmatrix}.$$

The transfer matrix is  $t(u) = \text{tr}T(u) = A(u) + D(u)$ .

## II. Heisenberg Chains: With $U(1)$ -symmetry

Periodic boundary condition

The R-matrix satisfies the Yang-Baxter equation (YBE)

$$R_{12}(u-v) R_{13}(u) R_{23}(v) = R_{23}(v) R_{13}(u) R_{12}(u-v). \quad (1)$$

The above fundamental relation leads to the following so-called RLL relation between the monodromy matrix

$$R_{00'}(u-v) T_0(u) T_{0'}(v) = T_{0'}(v) T_0(u) R_{00'}(u-v). \quad (2)$$

This leads to

$$[t(u), t(v)] = 0, \quad (3)$$

which ensures the integrability of the Heisenberg chain with periodic boundary condition.



## II. Heisenberg Chains: With $U(1)$ -symmetry

Periodic boundary condition

The eigenvalue  $\Lambda(u)$  of the transfer matrix  $t(u)$  can be parameterized by some parameters  $\{\lambda_1, \dots, \lambda_M | M = 0, \dots, N\}$  as follows (H. Bethe, Z. Phys. 71, 205 (1931)):

$$\Lambda(u) = a(u) \frac{Q(u - \eta)}{Q(u)} + d(u) \frac{Q(u + \eta)}{Q(u)}, \quad (4)$$

where

$$a(u) = \prod_{l=1}^N (u - \theta_l + \eta) = d(u + \eta), \quad Q(u) = \prod_{j=1}^M (u - \lambda_j),$$

the parameters  $\{\lambda_i\}$  should satisfy Bethe ansatz equations,

$$\prod_{k \neq j}^M \frac{\lambda_j - \lambda_k + \eta}{\lambda_j - \lambda_k - \eta} = \prod_{l=1}^N \frac{\lambda_j - \theta_l + \eta}{\lambda_j - \theta_l}, \quad j = 1, \dots, M.$$

## II. Heisenberg Chains: With $U(1)$ -symmetry

Periodic boundary condition

It can be proven that the transfer matrix  $t(u)$  satisfies the relations:

$$t(\theta_j) t(\theta_j - \eta) = a(\theta_j) d(\theta_j - \eta), \quad j = 1, \dots, N, \quad (5)$$

$$t(u) = 2u^N \times \text{id} + \dots, \quad u \rightarrow \infty. \quad (6)$$

This leads to that the eigenvalues  $\Lambda(u)$  satisfy the corresponding relations:

$$\Lambda(\theta_j) \Lambda(\theta_j - \eta) = a(\theta_j) d(\theta_j - \eta), \quad j = 1, \dots, N, \quad (7)$$

$$\Lambda(u) = 2u^N + \dots, \quad u \rightarrow \infty. \quad (8)$$

## II. Heisenberg Chains: With $U(1)$ -symmetry

With parallel boundary fields

The Hamiltonian of the Heisenberg chain with parallel boundary fields is

$$H = \sum_{k=1}^{N-1} \left( \sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y + \sigma_k^z \sigma_{k+1}^z \right) + \frac{\eta}{p} \sigma_1^z + \frac{\eta}{q} \sigma_N^z + N.$$

The system is **integrable**, i.e., the corresponding transfer matrix  $t(u)$  can be constructed by the R-matrix and the associated K-matrices

$$t(u) = \text{tr}(K^+(u) \mathcal{T}(u)) = \text{tr}(K^+(u) T(u) K^-(u) T^{-1}(-u)),$$

where the K-matrices  $K^\pm(u)$  are the diagonal K-matrices

$$K^-(u) = \begin{pmatrix} p+u & \\ & p-u \end{pmatrix}, \quad K^+(u) = \begin{pmatrix} q+u+\eta & \\ & q-u-\eta \end{pmatrix}.$$

The K-matrix  $K^-(u)$  satisfies the reflection equation (RE)

$$\begin{aligned} R_{12}(u_1 - u_2) K_1^-(u_1) R_{21}(u_1 + u_2) K_2^-(u_2) \\ = K_2^-(u_2) R_{12}(u_1 + u_2) K_1^-(u_1) R_{21}(u_1 - u_2), \end{aligned}$$

while the dual K-matrix  $K^+(u)$  satisfies the following dual RE

$$\begin{aligned} R_{12}(u_2 - u_1) K_1^+(u_1) R_{21}(-u_1 - u_2 - 2) K_2^+(u_2) \\ = K_2^+(u_2) R_{12}(-u_1 - u_2 - 2) K_1^+(u_1) R_{21}(u_2 - u_1). \end{aligned}$$

## II. Heisenberg Chains: With $U(1)$ -symmetry

With parallel boundary fields

The eigenvalues of the associated transfer matrix is also given in terms of a  $T - Q$  relation (E.K. Sklyanin, J. Phys. A 21, 2375 (1988))

$$\Lambda(u) = a(u) \frac{Q(u - \eta)}{Q(u)} + d(u) \frac{Q(u + \eta)}{Q(u)},$$

where

$$a(u) = \frac{2(u + \eta)}{2u + \eta} (u + p)(u + q) \prod_{l=1}^N (u - \theta_l + \eta)(u + \theta_l + \eta),$$

$$d(u) = a(-u - \eta), \quad Q(u) = \prod_{j=1}^M (u - \lambda_j)(u + \lambda_j + \eta).$$

## II. Heisenberg Chains: With $U(1)$ -symmetry

Universal properties of Heisenberg Chains with  $U(1)$ -symmetry

The eigenvalue can be given in terms of a homogeneous  $T - Q$  relation

$$\Lambda(u) = a(u) \frac{Q(u - \eta)}{Q(u)} + d(u) \frac{Q(u + \eta)}{Q(u)}, \quad (9)$$

where the roots of  $Q(u)$  satisfy the Bethe ansatz equations (BAEs)

$$\frac{a(\lambda_j)}{d(\lambda_j)} = - \frac{Q(\lambda_j + \eta)}{Q(\lambda_j - \eta)}, \quad j = 1, \dots, M. \quad (10)$$

BAEs  $\Rightarrow$  TBA

## II. Heisenberg Chain: Without $U(1)$ -symmetry

With unparallel boundary fields

The Hamiltonian of the Heisenberg chain with unparallel boundary fields is

$$H = \sum_{k=1}^{N-1} \left( \sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y + \sigma_k^z \sigma_{k+1}^z \right) + \frac{\eta}{p} \sigma_1^z + \frac{\eta}{q} (\sigma_N^z + \xi \sigma_N^x) + N. \quad (11)$$

The system is **integrable**, i.e., the corresponding transfer matrix  $t(u)$  can be constructed by the R-matrix and the associated K-matrices

$$t(u) = \text{tr}(K^+(u) \mathcal{T}(u)) = \text{tr}(K^+(u) \mathcal{T}(u) K^-(u) \mathcal{T}^{-1}(-u)),$$

where the K-matrices  $K^\pm(u)$  are the diagonal K-matrices

$$K^-(u) = \begin{pmatrix} p+u & \\ & p-u \end{pmatrix}, \quad K^+(u) = \begin{pmatrix} q+u+\eta & \xi(u+\eta) \\ \xi(u+\eta) & q-u-\eta \end{pmatrix}.$$

$$H = \eta \frac{\partial}{\partial u} \ln t(u) \Big|_{u=0, \{\theta_j\}=0}.$$

Without losing generality, we set  $\eta = i$ .

## II. Heisenberg Chains: Without $U(1)$ -symmetry

With unparallel boundary fields

The eigenvalue  $\Lambda(u)$  satisfies the properties (J. Cao et al, Nucl. Phys. B 875 (2013), 152-165):

$$\Lambda(-u - \eta) = \Lambda(u), \quad (12)$$

$$\Lambda(0) = 2pq \prod_{l=1}^N (1 - \theta_l)(1 + \theta_l), \quad (13)$$

$$\lim_{u \rightarrow \infty} \Lambda(u) = 2u^{2N+2} + \dots, \quad (14)$$

$$\Lambda(\theta_j)\Lambda(\theta_j - \eta) = -\frac{\Delta_q(\theta_j)}{(2\theta_j + \eta)(2\theta_j - \eta)}, \quad j = 1, \dots, N, \quad (15)$$

where the quantum determinant  $\Delta_q(u)$  is given by

$$\Delta_q(u) = 4(u^2 - 1)(p^2 - u^2)((1 + \xi^2)u^2 - q^2) \prod_{l=1}^N ((u - 1)^2 - \theta_l^2)((u + 1)^2 - \theta_l^2).$$

## II. Heisenberg Chains: Without $U(1)$ -symmetry

With unparallel boundary fields: Eigenvalues

The eigenvalue  $\Lambda(u)$  of the corresponding transfer matrix is given in terms of an inhomogeneous  $T - Q$  relation

$$\begin{aligned}\Lambda(u) &= a(u) \frac{Q(u-\eta)}{Q(u)} + d(u) \frac{Q(u+\eta)}{Q(u)} \\ &\quad + 2 \left[ 1 - (1 + \xi^2)^{\frac{1}{2}} \right] u(u+\eta) \frac{a(u)d(u)}{Q(u)},\end{aligned}\tag{16}$$

where

$$\begin{aligned}a(u) &= \frac{2(u+\eta)}{2u+\eta} (u+p) [(1 + \xi^2)^{\frac{1}{2}} u + q] \prod_{l=1}^N (u - \theta_l + \eta)(u + \theta_l + \eta), \\ d(u) &= a(-u - \eta), \quad Q(u) = \prod_{j=1}^N (u - \lambda_j)(u + \lambda_j + \eta).\end{aligned}$$

The roots of  $Q(u)$  satisfy the BAEs

$$\frac{a(\lambda_j)}{d(\lambda_j)} + \frac{Q(\lambda_j + \eta)}{Q(\lambda_j - \eta)} = -2 \left[ 1 - (1 + \xi^2)^{\frac{1}{2}} \right] \lambda_j (\lambda_j + \eta) \frac{a(\lambda_j)}{Q(\lambda_j - \eta)}, \quad j = 1, \dots, N.\tag{17}$$



### III. Thermodynamic limit of the Heisenberg spin chain

With non-diagonal boundary terms I

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The eigenvalue  $\Lambda(u)$  of the corresponding transfer matrix is given in terms of an inhomogeneous  $T - Q$  relation

$$\begin{aligned}\Lambda(u) = & \frac{2(u+1)^{2N+1}}{2u+1} (u+p) \left[ (1+\xi^2)^{\frac{1}{2}} u + q \right] \frac{Q(u-1)}{Q(u)} \\ & + \frac{2u^{2N+1}}{2u+1} (u-p+1) \left[ (1+\xi^2)^{\frac{1}{2}} (u+1) - q \right] \frac{Q(u+1)}{Q(u)} \\ & + 2 \left[ 1 - (1+\xi^2)^{\frac{1}{2}} \right] \frac{[u(u+1)]^{2N+1}}{Q(u)},\end{aligned}\tag{18}$$

where the function  $Q(u)$  can be parameterized as  $Q(u) = \prod_{j=1}^N (u - \lambda_j)(u + \lambda_j + 1)$ .

### III. Thermodynamic limit of the Heisenberg spin chain

With non-diagonal boundary terms I

- Bethe ansatz equations

$$\begin{aligned} \left(\frac{\lambda_j + 1}{\lambda_j}\right)^{2N+1} \frac{(\lambda_j + \rho) \left[(1 + \xi^2)^{\frac{1}{2}} \lambda_j + q\right]}{(\lambda_j - \rho + 1) \left[(1 + \xi^2)^{\frac{1}{2}} (\lambda_j + 1) - q\right]} = \\ - \frac{\left[1 - (1 + \xi^2)^{\frac{1}{2}}\right] (2\lambda_j + 1)(\lambda_j + 1)^{2N+1}}{(\lambda_j - \rho + 1) \left[(1 + \xi^2)^{\frac{1}{2}} (\lambda_j + 1) - q\right] \prod_{l=1}^N (\lambda_j - \lambda_l - 1)(\lambda_j + \lambda_l)} \\ - \prod_{l=1}^N \frac{(\lambda_j - \lambda_l + 1)(\lambda_j + \lambda_l + 2)}{(\lambda_j - \lambda_l - 1)(\lambda_j + \lambda_l)}, \quad j = 1, \dots, N. \end{aligned} \quad (19)$$

- The eigenvalue of the Hamiltonian

$$E = \sum_{j=1}^N \frac{2}{\lambda_j(\lambda_j + 1)} + N - 1 + \frac{1}{\rho} + \frac{(1 + \xi^2)^{\frac{1}{2}}}{q}. \quad (20)$$

### III. Thermodynamic limit of the Heisenberg spin chain

With non-diagonal boundary terms I

We define the contribution of the inhomogeneous term to the ground state energy as

$$E_{inh} = E_{hom} - E_{true}. \quad (21)$$

Here  $E_{hom}$  is the ground state energy of the Heisenberg chain calculated by the homogeneous  $T - Q$  relation

$$\begin{aligned} \Lambda_{hom}(u) &= \frac{2(u+1)^{2N+1}}{2u+1} (u+p) \left[ (1+\xi^2)^{\frac{1}{2}} u + q \right] \frac{Q(u-1)}{Q(u)} \\ &\quad + \frac{2u^{2N+1}}{2u+1} (u-p+1) \left[ (1+\xi^2)^{\frac{1}{2}} (u+1) - q \right] \frac{Q(u+1)}{Q(u)}. \end{aligned} \quad (22)$$

The singular property of the  $T - Q$  relation (22) gives the following BAEs

$$\left( \frac{\mu_j - \frac{i}{2}}{\mu_j + \frac{i}{2}} \right)^{2N} \frac{(\mu_j - i\bar{p})(\mu_j - i\bar{q})}{(\mu_j + i\bar{p})(\mu_j + i\bar{q})} = \prod_{l \neq j}^M \frac{(\mu_j - \mu_l - i)(\mu_j + \mu_l - i)}{(\mu_j - \mu_l + i)(\mu_j + \mu_l + i)}, \quad (23)$$

where we have put  $\lambda = i\mu - \frac{1}{2}$ ,  $\bar{p} = p - \frac{1}{2}$  and  $\bar{q} = q(1 + \xi^2)^{-\frac{1}{2}} - \frac{1}{2}$ . Note,  $E_{hom}$  is given by equation (20) with the constraint (23).

### III. Thermodynamic limit of the Heisenberg spin chain

With non-diagonal boundary terms I

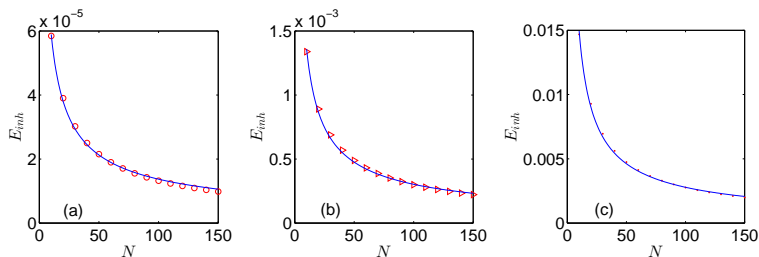


Figure 1: The contribution of the inhomogeneous term to the ground state energy  $E_{inh}$  versus the system size  $N$ . The data can be fitted as  $E_{inh} = \gamma_1 N^{\beta_1}$ . Due to the fact  $\beta_1 < 0$ , when the  $N$  tends to infinity, the contribution of the inhomogeneous term tends to zero. Here  $p = 8$ ,  $q = 4$ , (a)  $\xi = \frac{1}{8}$ ,  $\gamma_1 = 0.000253$  and  $\beta_1 = -0.6334$ ; (b)  $\xi = \frac{5}{8}$ ,  $\gamma_1 = 0.006096$  and  $\beta_1 = -0.6521$ ; (c)  $\xi = \frac{25}{8}$ ,  $\gamma_1 = 0.080180$  and  $\beta_1 = -0.7297$ .

### III. Thermodynamic limit of the Heisenberg spin chain

With non-diagonal boundary terms I

- Boundary energy

$$\begin{aligned} E_b(p, q, \xi) &= \lim_{N \rightarrow \infty} \left[ E_0(N; p, q, \xi) - 2E_0^{\text{periodic}}(N) \right] \\ &= -2 \int_0^\infty \frac{e^{-p\omega}}{1 + e^{-\omega}} d\omega - 2 \int_0^\infty \frac{e^{-\frac{q}{\sqrt{1+\xi^2}}\omega}}{1 + e^{-\omega}} d\omega \\ &\quad + \pi - 2 \ln 2 - 1 + \frac{1}{p} + \frac{(1 + \xi^2)^{\frac{1}{2}}}{q}. \end{aligned} \tag{24}$$

### III. Thermodynamic limit of the Heisenberg spin chain

With non-diagonal boundary terms I

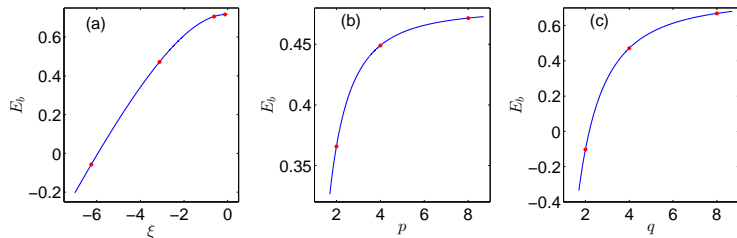


Figure 2: The boundary energies versus the boundary parameters. The blue curves are the ones calculated from equation (24), while the red points are the ones obtained from the Hamiltonian (11) with the BST algorithms. Here (a)  $p = 8$  and  $q = 4$ ; (b)  $q = 4$  and  $\xi = -\frac{25}{8}$ ; (c)  $p = 8$  and  $\xi = -\frac{25}{8}$ .

### III. Thermodynamic limit of the Heisenberg spin chain

With non-diagonal boundary terms I

When  $\xi$  is small, we can expand the boundary energy (24) with respect to  $\xi$  as

$$\begin{aligned} E_b(p, q, \xi) &\simeq \frac{1}{p} + \psi^{(0)}\left(\frac{p}{2}\right) - \psi^{(0)}\left(\frac{p+1}{2}\right) + \frac{1}{q} + \psi^{(0)}\left(\frac{q}{2}\right) - \psi^{(0)}\left(\frac{q+1}{2}\right) \\ &+ \pi - 1 - 2 \ln(2) + \xi^2 \left[ \frac{1}{2q} - \frac{1}{4} q \psi^{(1)}\left(\frac{q}{2}\right) + \frac{1}{4} q \psi^{(1)}\left(\frac{q+1}{2}\right) \right] \\ &+ \xi^4 \frac{\left[ q^3 \psi^{(2)}\left(\frac{q}{2}\right) - q^3 \psi^{(2)}\left(\frac{q+1}{2}\right) + 6q^2 \psi^{(1)}\left(\frac{q}{2}\right) - 6q^2 \psi^{(1)}\left(\frac{q+1}{2}\right) - 4 \right]}{32q} \\ &+ O(\xi^6), \end{aligned} \tag{25}$$

where  $\psi^{(m)}(x)$  is the  $m$ -order derivative of digamma function. Up to the order  $\xi^2$ , our result coincides with that of R. Nepomechie, J. Phys. A 46 (2013), 442002.

### III. Thermodynamic limit of the Heisenberg spin chain

With non-diagonal boundary terms II

The eigenvalue  $\Lambda(u)$  satisfies the properties (J. Cao et al, Nucl. Phys. B 875 (2013), 152-165):

$$\Lambda(-u - \eta) = \Lambda(u), \quad (26)$$

$$\Lambda(0) = 2pq \prod_{l=1}^N (\eta - \theta_l)(\eta + \theta_l), \quad (27)$$

$$\lim_{u \rightarrow \infty} \Lambda(u) = 2u^{2N+2} + \dots, \quad (28)$$

$$\Lambda(\theta_j)\Lambda(\theta_j - \eta) = -\frac{\Delta_q(\theta_j)}{(2\theta_j + \eta)(2\theta_j - \eta)}, \quad j = 1, \dots, N. \quad (29)$$



### III. Thermodynamic limit of the Heisenberg spin chain

With non-diagonal boundary terms II

In order to make the Hamiltonian (11) hermitian the boundary parameters have to be taken as follows:

$$p^* = -p, \quad q^* = -q, \quad \xi^* = \xi,$$

which leads to

$$(t(u))^\dagger = t(-u^*), \quad \Lambda^*(u) = \Lambda(-u^*).$$

This fact allows us to give the decomposition of  $\Lambda(u)$  for an eigenvalue of the transfer matrix

$$\begin{aligned} \Lambda(u) &= 2 \prod_{j=1}^{M_1} \left(u - \mu_j + \frac{\eta}{2}\right) \left(u + \mu_j + \frac{\eta}{2}\right) \\ &\quad \times \prod_{j=1}^{M_2} \left(u - z_j + \frac{\eta}{2}\right) \left(u + z_j + \frac{\eta}{2}\right) \left(u - z_j^* + \frac{\eta}{2}\right) \left(u + z_j^* + \frac{\eta}{2}\right) \\ &\quad \times \prod_{j=1}^{M_b} \left(u - \eta v_j + \frac{\eta}{2}\right) \left(u + \eta v_j + \frac{\eta}{2}\right), \end{aligned} \tag{30}$$

where  $\mu_j$  and  $v_j$  are real numbers,  $z_j^* \neq (\pm)z_k$ , and  $M_b + M_1 + 2M_2 = N + 1$ .

### III. Thermodynamic limit of the Heisenberg spin chain

With non-diagonal boundary terms II

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For the ground state for a large even  $N$ , the corresponding  $\Lambda(u)$  takes the decomposition

$$\begin{aligned}\Lambda(u) &= 2(u - \eta\nu + \frac{\eta}{2})(u + \eta\nu + \frac{\eta}{2}) \\ &\times \prod_{j=1}^{\frac{N}{2}} (u - x_j - \frac{\eta}{2})(u + x_j + \frac{3\eta}{2})(u - x_j + \frac{3\eta}{2})(u + x_j - \frac{\eta}{2}).\end{aligned}$$

This implies that  $z_j \simeq x_j \pm \eta$  for a large even  $N$  where  $x_j$  is a real number which corresponds to the position of the 2-string, and that  $\nu$  is a real number which is the position of a boundary bound state.

### III. Thermodynamic limit of the Heisenberg spin chain

With non-diagonal boundary terms II

The corresponding ground state energy  $E_0(N; P, Q, \xi)$  is expressed in terms of roots as

$$\begin{aligned}\lim_{N \rightarrow \infty} E_0(N; P, Q, \xi) &= \frac{1}{\frac{1}{4} - \nu^2} + \lim_{N \rightarrow \infty} \left\{ \sum_{j=1}^{\frac{N}{2}} \left( \frac{3}{x_j^2 + \frac{9}{4}} - \frac{1}{x_j^2 + \frac{1}{4}} \right) \right\} \\ &= \frac{1}{\frac{1}{4} - \nu^2} + \int_{-\infty}^{+\infty} \left( \frac{3}{x^2 + \frac{9}{4}} - \frac{1}{x^2 + \frac{1}{4}} \right) \rho(x) dx,\end{aligned}$$

where  $\rho(x)$  is the density of the distribution of roots.

Numerical study shows that inhomogeneous real parameters  $\{\theta_j\}$  almost does not affect the imaginary parts of the roots  $\{z_j\}$ . Namely,  $z_j \simeq x_j \pm \eta$ . This fact allows us to derive a linear integral equation of the density of the roots with an auxiliary density  $\sigma(\theta)$  of the inhomogeneities. Taking  $\sigma(\theta) = \delta(0)$  or the homogeneous limit and the value of  $\Lambda(0)$  allow us to determine  $\rho(x)$  and the real value  $\nu$ . Finally, we obtain the same expression (24) of the boundary energy  $E_b(p, q, \xi)$ .

## IV. Thermodynamic limit of other spin chains

The spin-1 Heisenberg spin chain

The Hamiltonian of the spin-1 Heisenberg chain with unparallel boundary fields is

$$\begin{aligned} H = & \frac{1}{\eta} \sum_{j=1}^{N-1} \left[ \vec{S}_j \cdot \vec{S}_{j+1} - (\vec{S}_j \cdot \vec{S}_{j+1})^2 \right] + \frac{1}{\eta} \left( 3N + \frac{8}{3} \right) \\ & + \frac{1}{\rho_-^2 - \frac{1}{4} (1 + \alpha_-^2)} \frac{1}{\eta^2} \left[ 2\rho_- (\alpha_- \cos \phi_- S_1^x - \alpha_- \sin \phi_- S_1^y + S_1^z) - \eta (S_1^z)^2 \right. \\ & - \frac{1}{2} \alpha_-^2 \eta \left[ \cos(2\phi_-) \left[ (S_1^x)^2 - (S_1^y)^2 \right] - (S_1^z)^2 \right] - \alpha_- \eta \cos \phi_- [S_1^x S_1^z + S_1^z S_1^x] \\ & \left. + \frac{1}{2} \alpha_-^2 \eta \sin(2\phi_-) [S_1^x S_1^y + S_1^y S_1^x] + \alpha_- \eta \sin \phi_- [S_1^y S_1^z + S_1^z S_1^y] + \eta h_1 \right] \\ & + \frac{1}{\rho_+^2 - \frac{1}{4} (1 + \alpha_+^2)} \frac{1}{\eta^2} \left[ 2\rho_+ (\alpha_+ \cos \phi_+ S_N^x - \alpha_+ \sin \phi_+ S_N^y - S_N^z) - \eta (S_N^z)^2 \right. \\ & - \frac{1}{2} \alpha_+^2 \eta \left[ \cos(2\phi_+) \left[ (S_N^x)^2 - (S_N^y)^2 \right] - (S_N^z)^2 \right] + \alpha_+ \eta \cos \phi_+ [S_N^x S_N^z + S_N^z S_N^x] \\ & \left. + \frac{1}{2} \alpha_+^2 \eta \sin(2\phi_+) [S_N^x S_N^y + S_N^y S_N^x] - \alpha_+ \eta \sin \phi_+ [S_N^y S_N^z + S_N^z S_N^y] + \eta h_N \right]. \end{aligned}$$



## IV. Thermodynamic limit of other spin chains

The spin-1 Heisenberg spin chain

The corresponding  $K$ -matrices  $K^{\pm(1)}(u)$  are the non-diagonal  $K$ -matrices

$$K_1^{+(1)}(u) = K_1^{- (1)}(-u - \eta)|_{(p_-, \alpha_-, \phi_-) \rightarrow (p_+, \alpha_+, \phi_+)},$$

$$K_1^{- (1)}(u) = (2u + \eta) \begin{pmatrix} x_1(u) & y_4'(u) & y_6'(u) \\ y_4(u) & x_2(u) & y_5'(u) \\ y_6(u) & y_5(u) & x_3(u) \end{pmatrix},$$

where the matrix elements are

$$x_1(u) = \left(p_- + u + \frac{\eta}{2}\right) \left(p_- + u - \frac{\eta}{2}\right) + \frac{\alpha_-^2}{2} \eta \left(u - \frac{\eta}{2}\right),$$

$$x_2(u) = \left(p_- + u - \frac{\eta}{2}\right) \left(p_- - u + \frac{\eta}{2}\right) + \alpha_-^2 \left(u + \frac{\eta}{2}\right) \left(u - \frac{\eta}{2}\right),$$

$$x_3(u) = \left(p_- - u - \frac{\eta}{2}\right) \left(p_- - u + \frac{\eta}{2}\right) + \frac{\alpha_-^2}{2} \eta \left(u - \frac{\eta}{2}\right),$$

$$y_4(u) = \sqrt{2} \alpha_- e^{-i\phi_-} u \left(p_- + u - \frac{\eta}{2}\right), \quad y_4'(u) = \sqrt{2} \alpha_- e^{i\phi_-} u \left(p_- + u - \frac{\eta}{2}\right),$$

$$y_5(u) = \sqrt{2} \alpha_- e^{-i\phi_-} u \left(p_- - u + \frac{\eta}{2}\right), \quad y_5'(u) = \sqrt{2} \alpha_- e^{i\phi_-} u \left(p_- - u + \frac{\eta}{2}\right),$$

$$y_6(u) = \alpha_-^2 e^{-2i\phi_-} u \left(u - \frac{\eta}{2}\right), \quad y_6'(u) = \alpha_-^2 e^{2i\phi_-} u \left(u - \frac{\eta}{2}\right).$$

## IV. Thermodynamic limit of other spin chains

The spin-1 Heisenberg spin chain

The eigenvalue  $\Lambda^{(1,1)}(u)$  of the transfer matrix  $t^{(1,1)}(u)$  satisfies the properties (J. Cao et al, JHEP 02 (2015), 036)

$$\Lambda^{(1,1)}(u) = \Lambda^{(1,1)}(-u - \eta), \quad \Lambda^{(\frac{1}{2},1)}(u) = \Lambda^{(\frac{1}{2},1)}(-u - \eta),$$

$$\Lambda^{(\frac{1}{2},1)}(0) = 2p_- p_+ \prod_{l=1}^N (\theta_l + \frac{3}{2}\eta)(-\theta_l + \frac{3}{2}\eta),$$

$$\Lambda^{(\frac{1}{2},1)}(u)|_{u \rightarrow \infty} = 2(\alpha_- \alpha_+ - 1)u^{2N+2} + \dots,$$

$$\Lambda^{(1,1)}(u)|_{u \rightarrow \infty} = 4[(1 + \alpha_+^2)(1 + \alpha_-^2) - 4(\alpha_+ \alpha_- - 1)^2]u^{4N+6} + \dots,$$

$$\Lambda^{(1,1)}(u) = -4u(u + \eta)\Lambda^{(\frac{1}{2},1)}\left(u + \frac{\eta}{2}\right)\Lambda^{(\frac{1}{2},1)}\left(u - \frac{\eta}{2}\right) + 4u(u + \eta)\delta^{(1)}\left(u + \frac{\eta}{2}\right),$$

$$\Lambda^{(1,1)}(\theta_j)\Lambda^{(\frac{1}{2},1)}\left(\theta_j - \frac{3\eta}{2}\right) = -4\theta_j(\theta_j + \eta)\delta^{(1)}\left(\theta_j - \frac{\eta}{2}\right)\Lambda^{(\frac{1}{2},1)}\left(\theta_j + \frac{\eta}{2}\right), \quad j = 1, \dots, N,$$

where  $\Lambda^{(\frac{1}{2},1)}(u)$  is the eigenvalue of a fundamental spin- $(\frac{1}{2}, 1)$  transfer matrix  $t^{(\frac{1}{2},1)}(u)$ .

## IV. Thermodynamic limit of other spin chains

### The spin-1 Heisenberg spin chain

This facts allows us to give the decomposition of  $\Lambda^{(1,1)}(u)$  and  $\Lambda^{(\frac{1}{2},1)}(u)$  for an eigenvalue of the transfer matrix

$$\Lambda^{(1,1)}(u) = \Lambda_0 \prod_{k=1}^{2N+3} \left( u - z_k^{(1)} + \frac{\eta}{2} \right) \left( u + z_k^{(1)} + \frac{\eta}{2} \right),$$
$$\Lambda^{(\frac{1}{2},1)}(u) = 2(\alpha_- \alpha_+ - 1) \prod_{l=1}^{N+1} \left( u - z_l + \frac{\eta}{2} \right) \left( u + z_l + \frac{\eta}{2} \right), \quad (31)$$

The energy spectrum of the Hamiltonian is determined by the zero roots  $\{z_j^{(1)}\}$  as

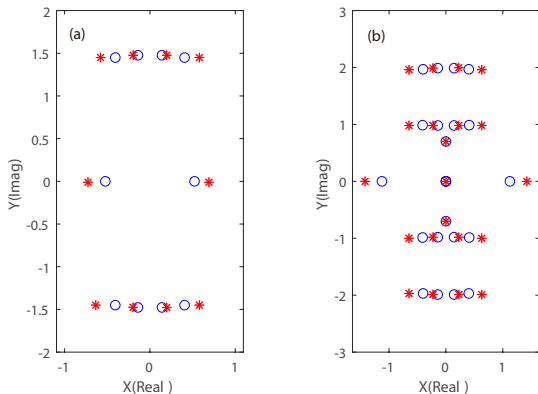
$$E = - \sum_{j=1}^{2N+3} \frac{\eta}{(z_j^{(1)})^2 - \frac{\eta^2}{4}}. \quad (32)$$

Without losing generality, we set  $\eta = 1$ .



## IV. Thermodynamic limit of other spin chains

The spin-1 Heisenberg spin chain



**Figure 3:** Exact numerical diagonalization results of the zero roots distributions at the ground state in parameter region E with  $N = 4$ ,  $p = 0.6$ ,  $q = -0.2$ . (a) the  $\bar{z}$ -roots of the eigenvalue  $\Lambda^{(\frac{1}{2}, 1)}(u)$ ; (b) the  $\bar{z}^{(1)}$ -roots of the eigenvalue  $\Lambda^{(1, 1)}(u)$ . The blue circles indicate the roots for  $\{\bar{\theta}_j = 0 | j = 1, \dots, 2N\}$  and the red asterisks specify the roots with the inhomogeneity parameters  $\{\bar{\theta}_j = 0.1(j - N - 0.5) | j = 1, \dots, 2N\}$ .

## IV. Thermodynamic limit of other spin chains

The spin-1 Heisenberg spin chain

The corresponding ground state energy  $E_0(N; p, q)$  is expressed in terms of roots as

$$\lim_{N \rightarrow \infty} E_0(N; p, q) = 4 + \frac{1}{\frac{1}{4} + z_0^2} + \frac{1}{\frac{1}{4} - (1 + |q|)^2} + \int_{-\infty}^{+\infty} \left( \frac{5}{x^2 + \frac{25}{4}} - \frac{1}{x^2 + \frac{1}{4}} \right) \rho(x) dx,$$

where  $p = \frac{p_+}{\sqrt{1+\alpha_+^2}} - \frac{1}{2}$ ,  $q = -\frac{p_-}{\sqrt{1+\alpha_-^2}} - \frac{1}{2}$  and  $z_0$  are real numbers.

Boundary energy  $E_b(N; p, q)$  is then given by

$$\begin{aligned} E_b(N; p, q) &= \lim_{N \rightarrow \infty} \left[ E_0(N; p, q) - 2E_0^{periodic}(N) \right] \\ &= \begin{cases} 2\pi - \frac{4}{3} + \frac{1}{p+1} - \frac{1}{p} + \frac{1}{q+1} - \frac{1}{q}, & p > 0, q > 0 \text{ or } q < -1 \\ 2\pi - \frac{4}{3} + \frac{1}{p+1} - \frac{1}{p} + \frac{1}{q+1} - \frac{1}{q} + 2\pi \csc(q\pi), & p > 0, -1 < p < 0 \end{cases} \end{aligned}$$



## IV. Thermodynamic limit of other spin chains

The Izergin-Korepin model

For the Izergin-Korepin model with unparallel boundary fields, the eigenvalue  $\Lambda(u)$  of the transfer matrix  $t(u)$  satisfies the properties (K. Hao et al, JHEP 06 (2014), 128)

$$\Lambda(u) = \Lambda(-u + 6\eta + i\pi),$$

$$\Lambda(\pm\theta_j)\Lambda(\pm\theta_j + 6\eta + i\pi) = \frac{\delta_1(u)}{\varphi_1(2u)} \Big|_{u=\pm\theta_j}, \quad j = 1, \dots, N,$$

$$\Lambda(\pm\theta_j)\Lambda(\pm\theta_j + 4\eta) = \frac{\delta_2(u) \times \Lambda(u + 2\eta + i\pi)}{\varphi_2(-2u + 8\eta)} \Big|_{u=\pm\theta_j}, \quad j = 1, \dots, N,$$

$$\lim_{u \rightarrow \pm\infty} \Lambda(u) = \left(\frac{1}{2}\right)^{2N} e^{\pm 2(N+1)(u-3\eta) - \varepsilon - \varepsilon'} [1 + 2 \cosh(\zeta' - \zeta + 2\eta)] + \dots,$$

$$\Lambda(0) = \Lambda(6\eta + i\pi) = (1 + 2e^{-\varepsilon} \sinh \eta) \text{tr}\{K^+(0)\} \prod_{l=1}^N \varphi_1(-\theta_l),$$

$$\Lambda(i\pi) = \Lambda(6\eta) = (1 - 2e^{-\varepsilon} \sinh \eta) \text{tr}\{K^+(i\pi)\} \prod_{l=1}^N \varphi_1(i\pi - \theta_l).$$

## IV. Thermodynamic limit of other spin chains

The Izergin-Korepin model

This facts also allows us to give the decomposition of  $\Lambda(u)$  for an eigenvalue of the transfer matrix

$$\Lambda(u) = \Lambda_0 \prod_{j=1}^{2N+2} \sinh\left(\frac{u}{2} - \frac{z_j}{2} - \frac{3\eta}{2}\right) \sinh\left(\frac{u}{2} + \frac{z_j}{2} - \frac{3\eta}{2} + \frac{i\pi}{2}\right). \quad (33)$$

The energy spectrum of the Hamiltonian is determined by the zero roots  $\{z_j\}$  as

$$E = - \sum_{j=1}^{2N+2} \left[ \frac{\sinh(3\eta)}{\cosh(3\eta) - \cos(iz_j)} + \frac{\sinh(3\eta)}{\cosh(3\eta) - \cos(iz_j + i\pi)} \right]. \quad (34)$$

# IV. Thermodynamic limit of other spin chains

The Izergin-Korepin model

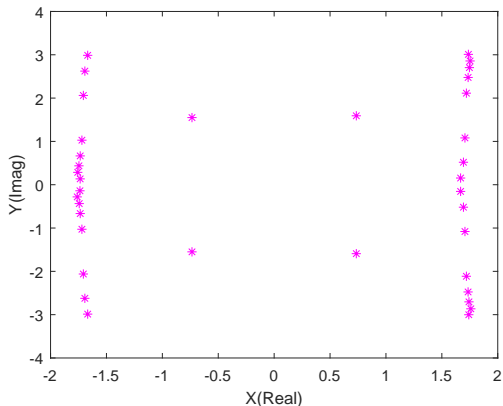


Figure 4: Exact numerical diagonalization results of the zero roots distributions at the ground state with  $N = 8$ ,  $\xi = 1$ ,  $\xi' = 0.6$  and  $\zeta' = 0.7$ .

# IV. Thermodynamic limit of other spin chains

The Izergin-Korepin model

The corresponding ground state energy  $E_0(N; p, q)$  is expressed in terms of roots as

$$\lim_{N \rightarrow \infty} E_0(N; \alpha, \alpha') = 2N \sum_{k=-\infty}^{\infty} [\tilde{a}_2(k) - \tilde{a}_8(k)e^{-i\pi k}] \tilde{\rho}(k),$$

where  $\tilde{a}_n(k) = e^{-\eta|nk|}$  is the Fourier transformation of  $a_n(u) = \frac{1}{2\pi} \frac{\sinh(n\eta)}{\cosh(n\eta) - \cos u}$  and  $\tilde{\rho}(k)$  is the Fourier transformation of the density  $\rho(z)$ .

$$\begin{aligned} \tilde{\rho}(k) = & [2N(\tilde{b}_4 + \tilde{b}_6 e^{-i\pi k})\tilde{\sigma}(k) + \tilde{b}_{|1+\frac{\alpha}{\eta}|} + \tilde{b}_{|1+\frac{\alpha'}{\eta}|} + \tilde{b}_6 - \tilde{b}_2 + 2(\tilde{b}_1 - \tilde{b}_3) \cos(\frac{\pi k}{2}) \\ & + (\tilde{b}_{|1-\frac{\alpha}{\eta}|} + \tilde{b}_{|1-\frac{\alpha'}{\eta}|} + \tilde{b}_6 - \tilde{b}_2)e^{-i\pi k}] / [2N(\tilde{b}_2 + \tilde{b}_8 e^{-i\pi k})], \end{aligned}$$

( $\ln \frac{\alpha}{\eta} = \operatorname{arcsinh}(\frac{e^\varepsilon}{2}) \geq 3$  and  $\frac{\alpha'}{\eta} = \operatorname{arcsinh}(\frac{e^{\varepsilon'}}{2}) \geq 3$  parameter region)

# IV. Thermodynamic limit of other spin chains

The Izergin-Korepin model

- Boundary energy ( $\ln \frac{\alpha}{\eta} = \operatorname{arcsinh}(\frac{e^\varepsilon}{2}) \geq 3$  and  $\frac{\alpha'}{\eta} = \operatorname{arcsinh}(\frac{e^{\varepsilon'}}{2}) \geq 3$  parameter region)

$$E_b(\alpha, \alpha') = e_b(\alpha) + e_b(\alpha') + e_{b0},$$

$$e_b(\alpha) = \sum_{k=-\infty}^{\infty} [1 - e^{-\eta|6k|-i\pi k}] \frac{e^{-\eta|(1+\frac{\alpha}{\eta})k|} + e^{-\eta|(1-\frac{\alpha}{\eta})k|-i\pi k}}{1 + e^{-\eta|6k|-i\pi k}},$$

$$e_b(\alpha') = \sum_{k=-\infty}^{\infty} [1 - e^{-\eta|6k|-i\pi k}] \frac{e^{-\eta|(1+\frac{\alpha'}{\eta})k|} + e^{-\eta|(1-\frac{\alpha'}{\eta})k|-i\pi k}}{1 + e^{-\eta|6k|-i\pi k}},$$

$$e_{b0} = \sum_{k=-\infty}^{\infty} [1 - e^{-\eta|6k|-i\pi k}] \frac{(e^{-\eta|6k|} - e^{-\eta|2k|})(1 + e^{-i\pi k}) + 2(e^{-\eta|k|} - e^{-\eta|3k|}) \cos \frac{\pi k}{2}}{1 + e^{-\eta|6k|-i\pi k}}.$$



## V. Conclusion and comments

So far, many typical  $U(1)$ -symmetry-broken models have been solved by the method:

- The spin- $\frac{1}{2}$  Heisenberg chain with arbitrary boundary fields.
- The open spin chains with general boundary condition associated with the  $A_n^{(1)}$  algebra.
- The t-J model with unparallel boundary fields.
- The Hubbard model with unparallel boundary fields.
- The open spin chains associated with the  $B_n^{(1)}$ ,  $C_n^{(1)}$  and  $D_n^{(1)}$  algebras.
- The open spin chains associated with the  $A_n^{(2)}$  and  $D_n^{(2)}$  twisted algebras.

Thanks for your attentions