

Off-diagonal approach to the exact solution of quantum integrable systems

Yi Qiao

Northwest University

Collaborators: Prof. Junpeng Cao, Prof. Wen-Li Yang...

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- Motivations
- XXX with closed boundary condition
 - Integrability
 - t-W scheme
 - Exact solution
 - Structure of roots
 - Explicit eigenfunctions of transfer matrix
- XXX with open boundary condition
- Summary

The eigenvalue problem of quantum integrable systems

- with $U(1)$ symmetry: coordinate Bethe Ansatz [1], $T - Q$ relation [2] and algebraic Bethe Ansatz [3, 4]...(homogeneous $T - Q$ relations)
- without $U(1)$ symmetry: fusion-based $T - Q$ relation [5], separation of variables [6, 7], modified algebraic Bethe ansatz [8] and off-diagonal Bethe ansatz[9, 10]...(inhomogeneous $T - Q$ relations)
- $t - W$ scheme [11, 12, 13]: BAEs are homogeneous; thermodynamic limit...

In the $t - W$ scheme, the W operator can be neglected in the thermodynamic limit, resulting in the $t - W$ relation becoming equivalent to the inversion relation [14, 15], but the exact proof is absent.

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| [2]. Baxter R J 1971 <i>Phys. Rev. Lett.</i> 26 832 | [10]. Wang Y, Yang W L, Cao J and Shi K 2015 <i>Off-diagonal Bethe ansatz for exactly solvable models</i> Springer, Berlin |
| [3]. Takhtadzhian L A and Faddeev L D 1979 <i>Russ. Math. Surv.</i> 34 11 | [11]. Qiao Y, Sun P, Cao J, Yang W L, Shi K and Wang Y 2020 <i>Phys. Rev. B</i> 102 085115 |
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- The Heisenberg spin chains with $U(1)$ -symmetry: With periodic boundary condition (PBC).
- The Heisenberg spin chains without $U(1)$ -symmetry: With nondiagonal boundary terms (nonparallel-OBC).

Integrability

I. Heisenberg spin chains with $U(1)$ -symmetry: Periodic boundary condition

The Heisenberg spin chain is a prototype quantum integrable model, whose Hamiltonian is

$$H^P = \sum_{n=1}^N (\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \sigma_n^z \sigma_{n+1}^z), \quad (1)$$

with the periodic boundary condition

$$\sigma_{N+1}^\alpha = \sigma_1^\alpha, \quad \alpha = x, y, z. \quad (2)$$

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

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

which may include $S^z = \frac{1}{2} \sum_{i=1}^N \sigma_i^z$.

Integrability

I. Heisenberg spin chains with $U(1)$ -symmetry: Periodic boundary condition

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

$$t(u) = \sum_{i=0}^N h_i u^i, \quad [t(u), t(v)] = [H, t(u)] = 0.$$

The eigenstates and the corresponding eigenvalues can be obtained by Quantum Inverse Scattering Method (QISM). In the framework of QISM, the monodromy matrix $T(u)$ has played a central role. It is built from the six-vertex R-matrix of

$$T_0(u) = R_{0N}(u - \theta_N) \dots R_{01}(u - \theta_1) = \begin{pmatrix} A(u) & B(u) \\ C(u) & D(u) \end{pmatrix}, \quad (3)$$

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

$$R(u) = \begin{pmatrix} u + \eta & & & \\ & u & \eta & \\ & \eta & u & \\ & & & u + \eta \end{pmatrix}. \quad (4)$$

The transfer matrix is

$$t(u) = \text{tr}\{T(u)\} = A(u) + D(u). \quad (5)$$

Integrability

I. Heisenberg spin chains with $U(1)$ -symmetry: Periodic boundary condition

The R -matrix has the following properties

$$\text{Initial condition : } R_{0,j}(0) = \eta P_{0,j},$$

$$\text{Unitary relation : } R_{0,j}(u)R_{j,0}(-u) = \phi(u) \times \text{id},$$

$$\text{Crossing relation : } R_{0,j}(u) = -\sigma_0^y R_{0,j}^{t_0}(-u - \eta)\sigma_0^y,$$

$$\text{PT-symmetry : } R_{0,j}(u) = R_{j,0}(u) = R_{0,j}^{t_0 t_j}(u),$$

$$\text{Z}_2\text{-symmetry : } \sigma_0^\alpha \sigma_j^\alpha R_{0,j}(u) = R_{0,j}(u)\sigma_0^\alpha \sigma_j^\alpha, \text{ for } \alpha = x, y, z,$$

$$\text{Fusion condition : } R_{0,j}(\pm\eta) = \eta(\pm 1 + P_{0,j}) = \pm 2\eta P_{0,j}^{(\pm)}, \quad (6)$$

where $\phi(u) = \eta^2 - u^2$, t_0 (or t_j) denotes the transposition in the space V_0 (or V_j), $P_{0,j}$ is the permutation operator. $P_{0,j}^{(-)}$ is the one-dimensional antisymmetric project operator defined in the one-dimensional subspace spanned by $\frac{1}{\sqrt{2}}(|12\rangle_{0,j} - |21\rangle_{0,j})$, $P_{0,j}^{(+)}$ is the three-dimensional symmetric projector defined in the three-dimensional subspace spanned by the orthogonal bases $\{|11\rangle_{0,j}, \frac{1}{\sqrt{2}}(|12\rangle_{0,j} + |21\rangle_{0,j}), |22\rangle_{0,j}\}$, $P_{0,j}^{(-)} + P_{0,j}^{(+)} = \text{id}$.

Integrability

I. Heisenberg spin chains with $U(1)$ -symmetry: Periodic boundary condition

The R-matrix (4) satisfies the [Yang-Baxter equation](#) (YBE)

$$R_{12}(u-v) R_{13}(u) R_{23}(v) = R_{23}(v) R_{13}(u) R_{12}(u-v). \quad (7)$$

The above fundamental relation leads to the following so-called [RTT relation](#) between the monodromy matrix

$$R_{0'0'}(u-v) T_0(u) T_{0'}(v) = T_{0'}(v) T_0(u) R_{0'0'}(u-v). \quad (8)$$

This leads to

$$[t(u), t(v)] = 0, \quad (9)$$

which ensures the integrability of the Heisenberg chain with periodic boundary condition (1)-(2) due to the fact that the Hamiltonian can be given in terms of the transfer matrix $t(u)$ as

$$H = 2\eta \frac{\partial}{\partial u} \ln t(u) \Big|_{u=0, \{\theta_j\}=0} - N, \quad [H, t(u)] = 0. \quad (10)$$

By using the **fusion technique**, we consider the product of transfer matrices $t(u)$ and $t(u - \eta)$

$$\begin{aligned} t(u)t(u - \eta) &= \text{tr}_{1,2} \{ T_2(u) T_1(u - \eta) \} \quad \text{[embedded into 2 auxiliary space]} \\ &= \text{tr}_{1,2} \left\{ T_2(u) T_1(u - \eta) (P_{1,2}^{(-)} + P_{1,2}^{(+)}) \right\} \\ &= \text{tr}_{1,2} \left\{ P_{1,2}^{(-)} T_2(u) T_1(u - \eta) P_{1,2}^{(-)} \right\} + \text{tr}_{1,2} \left\{ P_{1,2}^{(+)} T_2(u) T_1(u - \eta) P_{1,2}^{(+)} \right\} \\ &= a(u) d(u - \eta) \times \text{id} + d(u) \mathbb{W}(u), \quad \text{[extract constant } d(u) \text{ factor]} \end{aligned} \quad (11)$$

where the functions $a(u)$ and $d(u)$ are given by

$$a(u) = \prod_{j=1}^N (u - \theta_j + \eta), \quad d(u) = a(u - \eta), \quad (12)$$

$a(u)d(u - \eta)$ is the quantum determinant and $\mathbb{W}(u)$ is a new operator.

The detailed proof is as follows.

For **the first term** in the very relation (11): Starting from the YBE (7) with certain shift of spectral parameter, we obtain

$$R_{2,3}(u)R_{1,3}(u - \eta)P_{1,2}^{(-)} = P_{1,2}^{(-)}R_{2,3}(u)R_{1,3}(u - \eta)P_{1,2}^{(-)} = (u + \eta)(u - \eta) \times \text{id}. \quad (13)$$

We see that the fusion result of R -matrices with one-dimensional antisymmetric projector $P_{1,2}^{(-)}$ is a number. The fusion of monodromy matrices with $P_{1,2}^{(-)}$ gives

$$P_{1,2}^{(-)}T_2(u)T_1(u - \eta)P_{1,2}^{(-)} = a(u)d(u - \eta) \times \text{id}. \quad (14)$$

For the **second term** in the very relation (11): The fusion of R -matrices with the three-dimensional symmetric projector $P_{1,2}^{(+)}$ gives

$$P_{1,2}^{(+)} R_{2,3}(u) R_{1,3}(u - \eta) P_{1,2}^{(+)} = u \times R_{\{1,2\},3}^{(1, \frac{1}{2})}(u), \quad (15)$$

where $R_{\{1,2\},3}^{(1, \frac{1}{2})}(u)$ is the 6×6 fused R -matrix with the form of

$$R_{\{1,2\},3}^{(1, \frac{1}{2})}(u) = \begin{pmatrix} u + \eta & & & & & \\ & u - \eta & \sqrt{2}\eta & & & \\ \hline & \sqrt{2}\eta & u & & & \\ & & & u & \sqrt{2}\eta & \\ \hline & & & \sqrt{2}\eta & u - \eta & \\ & & & & & u + \eta \end{pmatrix}. \quad (16)$$

Then the fusion of monodromy matrices reads

$$P_{1,2}^{(+)} T_2(u) T_1(u - \eta) P_{1,2}^{(+)} = d(u) T_{\{1,2\}}^{(1, \frac{1}{2})}(u), \quad (17)$$

where $T_{\{1,2\}}^{(1, \frac{1}{2})}(u)$ is the fused monodromy matrix, which constructed by the fused R -matrix $R_{\{1,2\},j}^{(1, \frac{1}{2})}(u)$ as

$$T_{\{1,2\}}^{(1, \frac{1}{2})}(u) = R_{\{1,2\},N}^{(1, \frac{1}{2})}(u - \theta_N) \cdots R_{\{1,2\},1}^{(1, \frac{1}{2})}(u - \theta_1). \quad (18)$$

Then we arrive at that the $\mathbb{W}(u)$ operator in Eq.(11) is the fused transfer matrix as

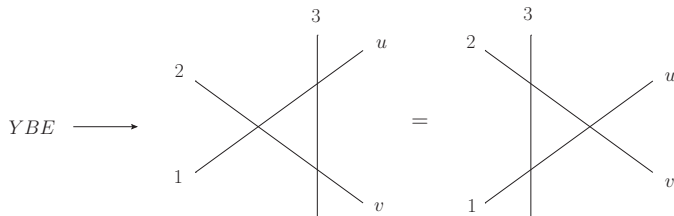
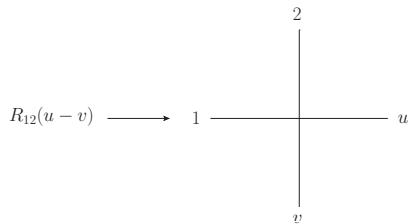
$$\mathbb{W}(u) = \text{tr}_{\{1,2\}} T_{\{1,2\}}^{(1, \frac{1}{2})}(u). \quad (19)$$

From the constructions (16) and (18), we know that the $\mathbb{W}(u)$ operator is a operator polynomial of u with the degrees N .

Graph Representation

R-matrix and the YBE

The fused R-matrix $R_{\{1,2\},3}^{(1,\frac{1}{2})}(u)$ also satisfy the YBE. To better understand the fusion procedure, we use a graph representation to illustrate it.



Graph Representation

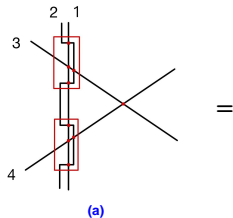
Proof of the YBE for the fused R-matrix

Recall
$$P_{1,2}^{(+)} R_{2,3}(u) R_{1,3}(u - \eta) P_{1,2}^{(+)} = u \times R_{\{1,2\},3}^{(1, \frac{1}{2})}(u).$$

Graph Representation

Proof of the YBE for the fused R-matrix

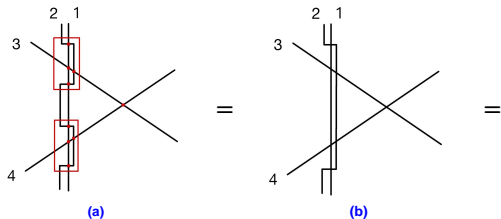
Recall $P_{1,2}^{(+)} R_{2,3}(u) R_{1,3}(u - \eta) P_{1,2}^{(+)} = u \times R_{\{1,2\},3}^{(1,\frac{1}{2})}(u).$



Graph Representation

Proof of the YBE for the fused R-matrix

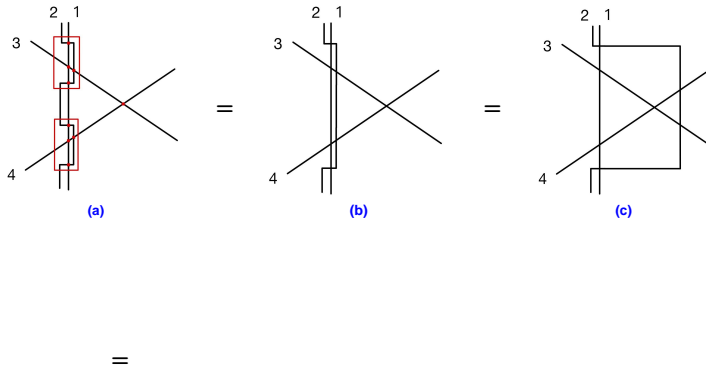
Recall $P_{1,2}^{(+)} R_{2,3}(u) R_{1,3}(u - \eta) P_{1,2}^{(+)} = u \times R_{\{1,2\},3}^{(1,\frac{1}{2})}(u).$



Graph Representation

Proof of the YBE for the fused R-matrix

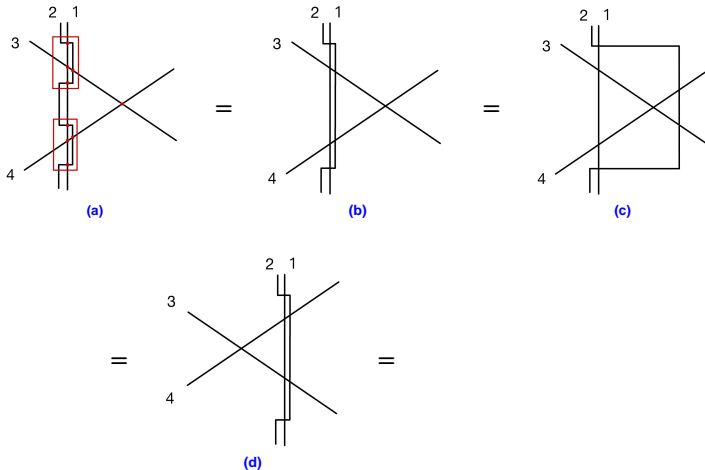
Recall $P_{1,2}^{(+)} R_{2,3}(u) R_{1,3}(u - \eta) P_{1,2}^{(+)} = u \times R_{\{1,2\},3}^{(1,\frac{1}{2})}(u).$



Graph Representation

Proof of the YBE for the fused R-matrix

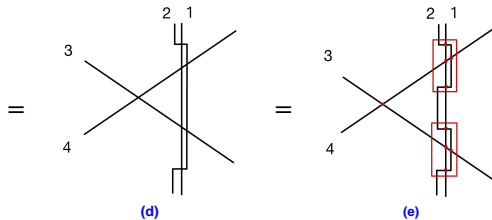
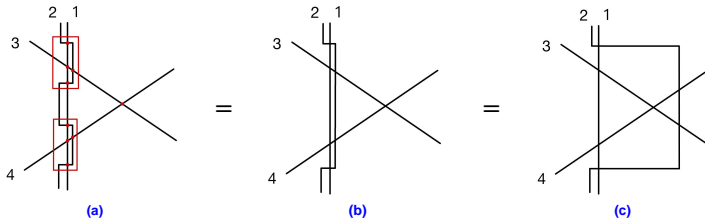
Recall $P_{1,2}^{(+)} R_{2,3}(u) R_{1,3}(u - \eta) P_{1,2}^{(+)} = u \times R_{\{1,2\},3}^{(1,\frac{1}{2})}(u).$



Graph Representation

Proof of the YBE for the fused R-matrix

Recall $P_{1,2}^{(+)} R_{2,3}(u) R_{1,3}(u - \eta) P_{1,2}^{(+)} = u \times R_{\{1,2\},3}^{(1,\frac{1}{2})}(u).$



$t - W$ scheme

I. Heisenberg spin chains with $U(1)$ -symmetry: Periodic boundary condition

At the points of $\{u = \theta_j\}$, the operator relation (11) can be simplified as

$$t(\theta_j)t(\theta_j - \eta) = a(\theta_j) d(\theta_j - \eta), \quad j = 1, \dots, N, \quad (20)$$

due to the fact $d(\theta_j) = 0$.

From the definition, we know that both $t(u)$ and $\mathbb{W}(u)$ are the operator-valued polynomial of u with degree N . Moreover, the matrices $t(u)$ and $\mathbb{W}(u)$ commute with each other, namely,

$$[t(u), t(v)] = [\mathbb{W}(u), \mathbb{W}(v)] = [t(u), \mathbb{W}(v)] = 0. \quad (21)$$

Thus they have common eigenstates. Acting the operator identities (11) and (20) on the common eigenstate $|\Psi\rangle$, we obtain [the \$t - W\$ relation](#)

$$\Lambda(u)\Lambda(u - \eta) = a(u) d(u - \eta) + d(u)W(u), \quad (22)$$

$$\Lambda(\theta_j)\Lambda(\theta_j - \eta) = a(\theta_j) d(\theta_j - \eta), \quad j = 1, \dots, N, \quad (23)$$

where $\Lambda(u)$ and $W(u)$ are the eigenvalues of the transfer matrix $t(u)$ and $\mathbb{W}(u)$ operator, respectively

$$t(u)|\Psi\rangle = \Lambda(u)|\Psi\rangle, \quad \mathbb{W}(u)|\Psi\rangle = W(u)|\Psi\rangle.$$

From the construction of transfer matrix (5), we conclude that

$$\Lambda(u), \text{ as a function of } u, \text{ is a polynomial of degree } N, \quad (24)$$

$$W(u), \text{ as a function of } u, \text{ is a polynomial of degree } N. \quad (25)$$

Meanwhile, $\Lambda(u)$ and $W(u)$ satisfy the asymptotic behaviors

$$\lim_{u \rightarrow \infty} \Lambda(u) = 2u^N + \dots, \quad \lim_{u \rightarrow \infty} W(u) = 3u^N + \dots. \quad (26)$$

Exact solution

I. Heisenberg spin chains with $U(1)$ -symmetry: Periodic boundary condition

In order to obtain the exact solution of the spin- $\frac{1}{2}$ XXX closed chain described by the Hamiltonian (1), let us take the homogeneous limit, i.e., $\{\theta_j = 0\}$. Usually, the eigenvalues $\Lambda(u)$ and $W(u)$ are expressed by the $T - Q$ relations with the help of Bethe roots. Here, we quantify the $\Lambda(u)$ and $W(u)$ by their zero roots as

$$\Lambda(u) = 2 \prod_{j=1}^N (u - z_j + \frac{\eta}{2}), \quad W(u) = 3 \prod_{j=1}^N (u - w_j), \quad (27)$$

where $\{z_j | j = 1, \dots, N\}$ and $\{w_j | j = 1, \dots, N\}$ are the zero roots of $\Lambda(u)$ and $W(u)$, respectively.

Substituting Eq.(27) with $\{u = z_j - \frac{\eta}{2}\}$ and $\{u = w_j\}$ into into the $t - W$ relation (22) with $\{\theta_j = 0\}$, we obtain that the zero roots $\{z_j\}$ and $\{w_j\}$ should satisfy the BAEs

$$(z_j + \frac{\eta}{2})^N (z_j - \frac{3}{2}\eta)^N = -(z_j - \frac{\eta}{2})^N W(z_j - \frac{\eta}{2}), \quad j = 1, \dots, N, \quad (28)$$

$$\Lambda(w_j) \Lambda(w_j - \eta) = (w_j + \eta)^N (w_j - \eta)^N, \quad j = 1, \dots, N. \quad (29)$$

Exact solution

I. Heisenberg spin chains with $U(1)$ -symmetry: Periodic boundary condition

The eigenvalues of the Hamiltonian (1) can be expressed in terms of the zero roots $\{z_j\}$ as

$$E^P = -2\eta \times \sum_{j=1}^N \frac{1}{z_j - \frac{\eta}{2}} - N. \quad (30)$$

For the finite system size N , one can solve the BAEs (28) and (29) numerically. Substituting the values of roots into Eq.(30), one obtains the energy of the system.

Structure of roots

I. Heisenberg spin chains with $U(1)$ -symmetry: Periodic boundary condition

We use the Hermitian property of the transfer matrix to analyse the structure of roots.

The R -matrix (4) has the **hermitian relation**

$$R_{0,j}^\dagger(u) = -R_{0,j}(-u^*). \quad (31)$$

Hermitian relation for the transfer matrix in the homogeneous limit:

$$\begin{aligned} t^\dagger(u) &= \text{tr}_0 \left\{ [R_{0,N}(u) \cdots R_{0,1}(u)]^\dagger \right\} \\ &= \text{tr}_0 \left\{ R_{0,1}^\dagger(u) \cdots R_{0,N}^\dagger(u) \right\} \\ &\stackrel{(31)}{=} (-1)^N \text{tr}_0 \left\{ R_{0,1}(-u^*) \cdots R_{0,N}(-u^*) \right\} \\ &= (-1)^N \text{tr}_0 \left\{ R_{0,N}^{t_0}(-u^*) \cdots R_{0,1}^{t_0}(-u^*) \right\} \\ &\stackrel{(6)}{=} \text{tr}_0 \left\{ \sigma_0^y R_{0,N}(u^* - \eta) \cdots R_{0,1}(u^* - \eta) \sigma_0^y \right\} \\ &= \text{tr}_0 \left\{ R_{0,N}(u^* - \eta) \cdots R_{0,1}(u^* - \eta) \right\} = t(u^* - \eta). \end{aligned} \quad (32)$$

Structure of roots

I. Heisenberg spin chains with $U(1)$ -symmetry: Periodic boundary condition

With the help of the $t - W$ relation (11), we find that the $\mathbb{W}(u)$ operator satisfies

$$\mathbb{W}^\dagger(u) = \mathbb{W}(u^*). \quad (33)$$

The relations (32) and (33) imply that the corresponding eigenvalues have the properties

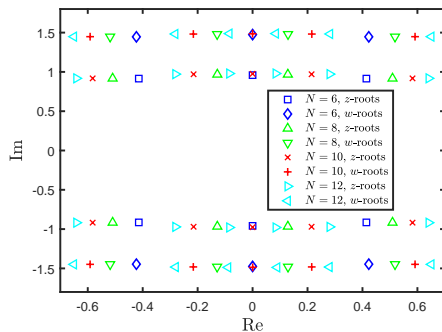
$$\Lambda^*(u) = \Lambda(u^* - \eta), \quad W^*(u) = W(u^*). \quad (34)$$

Combining the relations (34) and (22)-(27), we conclude that if z_j is the solution of $\Lambda(u)$, its complex conjugation z_j^* must be the solution, and if w_j is a solution of $W(u)$, the w_j^* must be the solution, which can be denoted as

$$\{z_j^*\} = \{z_j\}, \quad \{w_j^*\} = \{w_j\}. \quad (35)$$

Structure of roots

I. Heisenberg spin chains with $U(1)$ -symmetry: Periodic boundary condition



Patterns of zero roots at the ground state with $N = 6, 8, 10, 12$. The data are obtained by using the exact numerical diagonalization with the inhomogeneous parameters $\{\theta_j = 0\}$.

- The zero roots form the conjugate pairs around the line $\pm \frac{l\eta}{2}$ with a positive integer $l \geq 2$.
- At the ground state, z-roots and w-roots form the 2-strings with $l = 2, 3$ respectively.

Ground state eigenfunctions in the thermodynamic limit

I. Heisenberg spin chains with $U(1)$ -symmetry: Periodic boundary condition

Parameterization for the ground state:

- Denote the z -roots as $\{u_j^{(2)} \pm \eta | j = 1, \dots, N/2\}$, with $u_j^{(2)} \in \mathfrak{R}$.
- Denote the w -roots as $\{\bar{u}_j^{(2)} \pm \frac{3\eta}{2} | j = 1, \dots, N/2\}$, with $\bar{u}_j^{(2)} \in \mathfrak{R}$.

Substituting the parameterization into the expression of $\Lambda_g(u)$ and $W_g(u)$, we obtain

$$\Lambda_g(u) = 2 \prod_{j=1}^{N/2} (u - u_j^{(2)} - \frac{\eta}{2})(u - u_j^{(2)} + \frac{3\eta}{2}), \quad (36)$$

$$W_g(u) = 3 \prod_{j=1}^{N/2} (u - \bar{u}_j^{(2)} - \frac{3}{2}\eta)(u - \bar{u}_j^{(2)} + \frac{3}{2}\eta). \quad (37)$$

To analyze the leading terms of the eigenvalues, we define

$$\Lambda_g(u) = e^{N[\lambda_g^{(0)}(u) + \frac{1}{N}\lambda_g^{(1)}(u) + O(\frac{1}{N^2})]}, \quad (38)$$

$$W_g(u) = e^{N[\omega_g^{(0)}(u) + \frac{1}{N}\omega_g^{(1)}(u) + O(\frac{1}{N^2})]}, \quad (39)$$

where $\lambda_g^{(0)}(u)$ and $\omega_g^{(0)}(u)$ are the highest order terms of u , and $\lambda_g^{(1)}(u)$ and $\omega_g^{(1)}(u)$ are the second higher order terms.

Ground state eigenfunctions in the thermodynamic limit

I. Heisenberg spin chains with $U(1)$ -symmetry: Periodic boundary condition

In the thermodynamic limit $N \rightarrow \infty$, the leading terms of $\Lambda_g(u)$ can be obtained by taking the derivatives of logarithm of Eqs.(36) and (38)

$$\frac{\partial}{\partial u} \lambda_g^{(\beta)}(u) = \int_{-\infty}^{\infty} \left(\frac{1}{u - \lambda - \frac{\eta}{2}} + \frac{1}{u - \lambda + \frac{3\eta}{2}} \right) \rho_g^{(\beta)}(\lambda) d\lambda, \quad \beta = 0, 1, \quad (40)$$

where $\rho_g^{(\beta)}(\lambda)$ is the density of z -roots at the ground state. The leading terms of $W_g(u)$ are determined by taking the derivatives of logarithm of Eqs.(37) and (39) as

$$\frac{\partial}{\partial u} w_g^{(\beta)}(u) = \int_{-\infty}^{\infty} \left(\frac{1}{u - \lambda - \frac{3\eta}{2}} + \frac{1}{u - \lambda + \frac{\eta}{2}} \right) \rho_w^{(\beta)}(\lambda) d\lambda \quad \beta = 0, 1, \quad (41)$$

where $\rho_w^{(\beta)}(\lambda)$ is the density of w -roots.

The role of inset inhomogeneous parameters is to help us to determine the density of z -roots.

Take the difference of Eq.(23) at two nearest inhomogeneous points. In the thermodynamic limit, we set that the density of inhomogeneous parameters as the δ -function. Then we have

$$\frac{\partial}{\partial u} \ln[\Lambda_g(u)\Lambda_g(u - \eta)] = \frac{\partial}{\partial u} \ln[(u + \eta)^N(u - \eta)^N] + O\left(\frac{1}{N}\right), \quad (42)$$

where $O\left(\frac{1}{N}\right)$ is the order-dependent correction.

Ground state eigenfunctions in the thermodynamic limit

I. Heisenberg spin chains with $U(1)$ -symmetry: Periodic boundary condition

Substituting (38) into (42), we have

$$\begin{aligned}\frac{\partial}{\partial u} [\lambda_g^{(0)}(u) + \lambda_g^{(0)}(u - \eta)] &= \frac{1}{u + \eta} + \frac{1}{u - \eta}, & \lambda_g^{(0)}(0) &= 0, \\ \frac{\partial}{\partial u} [\lambda_g^{(1)}(u) + \lambda_g^{(1)}(u - \eta)] &= 0, & \lambda_g^{(1)}(0) &= 0.\end{aligned}\quad (43)$$

Substituting Eq.(40) with $\beta = 0$ into (43), we have

$$\int_{-\infty}^{\infty} \left(\frac{1}{u - \lambda - \frac{\eta}{2}} + \frac{1}{u - \lambda + \frac{\eta}{2}} + \frac{1}{u - \lambda - \frac{3\eta}{2}} + \frac{1}{u - \lambda + \frac{3\eta}{2}} \right) \rho_g^{(0)}(\lambda) d\lambda = \frac{1}{u + \eta} + \frac{1}{u - \eta}. \quad (44)$$

Solving Eq.(44) by the Fourier transformation, we obtain the solution of densities of z-roots as

$$\rho_g^{(0)}(\lambda) = \frac{1}{2 \cosh(\pi\lambda)}, \quad \rho_g^{(1)}(\lambda) = 0. \quad (45)$$

Using the energy expression (30) and the densities (45), we can directly determine the ground state energy in the thermodynamic limit

$$\begin{aligned}E_g &= -2Ni \int_{-\infty}^{\infty} \left(\frac{1}{\lambda + \frac{i}{2}} + \frac{1}{\lambda - \frac{3i}{2}} \right) (\rho_w^{(0)}(\lambda) + \rho_w^{(1)}(\lambda)) d\lambda - N \\ &= (1 - 4 \ln 2)N,\end{aligned}\quad (46)$$

which is consistent with the result obtained through algebraic Bethe ansatz [10].

Ground state eigenfunctions in the thermodynamic limit

I. Heisenberg spin chains with $U(1)$ -symmetry: Periodic boundary condition

Substituting Eq.(45) into (40) and taking the integral, we obtain

$$\lambda_g^{(0)}(u) = \ln \frac{2\Gamma(1 + \frac{i u}{2})\Gamma(\frac{3}{2} - \frac{i u}{2})}{\Gamma(\frac{1}{2} + \frac{i u}{2})\Gamma(1 - \frac{i u}{2})}, \quad \lambda_g^{(1)}(u) = 0. \quad (47)$$

The $\lambda_g^{(0)}(u)$ can be expanded with respect to u as

$$\lambda_g^{(0)}(u) = \ln u + \ln \frac{\cosh \frac{\pi u}{2}}{\sinh \frac{\pi u}{2}} + \frac{\eta}{2u} + \frac{1}{2u^2} + O(\frac{1}{u^2}), \quad \text{Im}(u) < 1. \quad (48)$$

From Eqs.(38), (47) and (48), we obtain that the eigenvalue of transfer matrix at the ground state with the thermodynamic limit is

$$\Lambda_g(u) = \left(\frac{2\Gamma(1 + \frac{i u}{2})\Gamma(\frac{3}{2} - \frac{i u}{2})}{\Gamma(\frac{1}{2} + \frac{i u}{2})\Gamma(1 - \frac{i u}{2})} \right)^N e^{O(\frac{1}{N})}. \quad (49)$$

Ground state eigenfunctions in the thermodynamic limit

I. Heisenberg spin chains with $U(1)$ -symmetry: Periodic boundary condition

Now, we calculate the leading terms of $W(u)$. Substituting $z_j = u_j^{(2)} + \frac{\eta}{2}$ into the BAEs (28), we obtain

$$(u_j^{(2)} + \frac{3\eta}{2})^N (u_j^{(2)} - \frac{\eta}{2})^N = -(u_j^{(2)} + \frac{\eta}{2})^N W_g(u_j^{(2)} + \frac{\eta}{2}), \quad j = 1, \dots, \frac{N}{2}, \quad (50)$$

where $\{u_j^{(2)}\}$ are real. Taking the complex conjugation of above relation, we have

$$(u_j^{(2)} + \frac{\eta}{2})^N (u_j^{(2)} - \frac{3\eta}{2})^N = -(u_j^{(2)} - \frac{\eta}{2})^N W_g(u_j^{(2)} - \frac{\eta}{2}), \quad j = 1, \dots, \frac{N}{2}. \quad (51)$$

Multiplying Eq.(50) with (51), we obtain

$$(u_j^{(2)} + \frac{3\eta}{2})^N (u_j^{(2)} - \frac{3\eta}{2})^N = W_g(u_j^{(2)} + \frac{\eta}{2}) W_g(u_j^{(2)} - \frac{\eta}{2}), \quad j = 1, \dots, \frac{N}{2}. \quad (52)$$

Taking the derivative of logarithm of above equation, we arrive at

$$\frac{1}{N} \frac{\partial}{\partial u} \ln[W_g(u + \frac{\eta}{2}) W_g(u - \frac{\eta}{2})] = \frac{1}{u + \frac{3\eta}{2}} + \frac{1}{u - \frac{3\eta}{2}} + O(\frac{1}{N^2}). \quad (53)$$

Ground state eigenfunctions in the thermodynamic limit

I. Heisenberg spin chains with $U(1)$ -symmetry: Periodic boundary condition

Substituting Eq.(39) into (53), we have

$$\begin{aligned}\frac{\partial}{\partial u} [w_g^{(0)}(u + \frac{\eta}{2}) + w_g^{(0)}(u - \frac{\eta}{2})] &= \frac{1}{u + \frac{3\eta}{2}} + \frac{1}{u - \frac{3\eta}{2}}, \\ \frac{\partial}{\partial u} [w_g^{(1)}(u + \frac{\eta}{2}) + w_g^{(1)}(u - \frac{\eta}{2})] &= 0.\end{aligned}\quad (54)$$

Substituting Eq.(41) into above equations and solving it by the Fourier transformation, we obtain the density of w -roots as

$$\rho_w^{(0)}(\lambda) = \frac{1}{2 \cosh(\pi\lambda)}, \quad \rho_w^{(1)}(\lambda) = 0. \quad (55)$$

Substituting Eq.(55) into (41), we have

$$\frac{\partial}{\partial u} w_g^{(0)}(u) = \frac{\partial}{\partial u} \ln \frac{\Gamma(\frac{3}{2} + \frac{i u}{2}) \Gamma(\frac{3}{2} - \frac{i u}{2})}{\Gamma(1 + \frac{i u}{2}) \Gamma(1 - \frac{i u}{2})} = \frac{\partial}{\partial u} \ln \left(\frac{(u + \eta)(u - \eta)}{2u} \tanh \frac{\pi u}{2} \right). \quad (56)$$

Taking the integration, we obtain

$$w_g^{(0)}(u) = \ln \left(\frac{C_w^{(0)}}{2} \frac{(u + \eta)(u - \eta)}{u} \tanh \frac{\pi u}{2} \right), \quad (57)$$

where $C_w^{(0)}$ is the integration constant.

Ground state eigenfunctions in the thermodynamic limit

I. Heisenberg spin chains with $U(1)$ -symmetry: Periodic boundary condition

Thus the ground state eigenvalue $W_g(u)$ can be expressed as

$$W_g(u) = \left(\frac{(u+\eta)(u-\eta)}{u} \right)^N \left(\frac{C_w^{(0)}}{2} \tanh \frac{\pi u}{2} \right)^N e^{\omega_g^{(1)}(0)} e^{O(\frac{1}{N})}. \quad (58)$$

Substituting Eq.(58) into the $t - W$ relation (22) with $\{\theta_j = 0\}$, we obtain

$$\begin{aligned} \Lambda_g(u)\Lambda_g(u-\eta) &= (u+\eta)^N(u-\eta)^N e^{O(\frac{1}{N})} \\ &= (u+\eta)^N(u-\eta)^N \left[1 + \left(\frac{C_w^{(0)}}{2} \tanh \frac{\pi u}{2} \right)^N C_w^{(1)} e^{O(\frac{1}{N})} \right]. \end{aligned} \quad (59)$$

When $u \rightarrow \infty$, from the asymptotic behavior of $\Lambda_g(u)$ or Eq.(49), we know that the coefficient of highest order term of left hand side of Eq.(59) is 4. In order to meet this constraint, the left hand side of Eq.(59) should also be 4, which gives that $C_w^{(0)} = 2$ and $C_w^{(1)} = 3$. Due to the fact that $\tanh \frac{\pi u}{2} < 1$, the second term of the right hand side of (59) turns to zero when $N \rightarrow \infty$, which gives that the W function can be neglected in the thermodynamic limit. Then we conclude that the $t - W$ relation (22) can be used to study the ground state physical properties.

Next, we consider the **open boundary condition**. The boundary reflections are characterized by the reflection matrices

$$K^-(u) = \begin{pmatrix} p+u & 0 \\ 0 & p-u \end{pmatrix}, \quad K^+(u) = \begin{pmatrix} q+u+\eta & \xi(u+\eta) \\ \xi(u+\eta) & q-u-\eta \end{pmatrix}, \quad (60)$$

which satisfy the reflection equation (RE)

$$R_{1,2}(\lambda-u)K_1^-(\lambda)R_{2,1}(\lambda+u)K_2^-(u) = K_2^-(u)R_{1,2}(\lambda+u)K_1^-(\lambda)R_{2,1}(\lambda-u), \quad (61)$$

and the dual reflection equation

$$\begin{aligned} & R_{1,2}(-\lambda+u)K_1^+(\lambda)R_{2,1}(-\lambda-u-2\eta)K_2^+(u) \\ &= K_2^+(u)R_{1,2}(-\lambda-u-2\eta)K_1^+(\lambda)R_{2,1}(-\lambda+u). \end{aligned} \quad (62)$$

Due to the boundary reflection, we should introduce the reflecting monodromy matrix

$$\hat{T}_0(u) = R_{0,1}(u+\theta_1)R_{0,2}(u+\theta_2)\cdots R_{0,N}(u+\theta_N). \quad (63)$$

The double-row monodromy matrix $\mathcal{U}_0(u)$ is

$$\mathcal{U}_0(u) = T_0(u)K_0^-(u)\hat{T}_0(u), \quad (64)$$

which satisfies the RE

$$R_{1,2}(\lambda - u)\mathcal{U}_1(\lambda)R_{2,1}(\lambda + u)\mathcal{U}_2(u) = \mathcal{U}_2(u)R_{1,2}(\lambda + u)\mathcal{U}_1(\lambda)R_{2,1}(\lambda - u). \quad (65)$$

The transfer matrix for the open boundary case is constructed as

$$t^\circ(u) = \text{tr}_0\{K_0^+(u)\mathcal{U}_0(u)\}. \quad (66)$$

The YBE and RE lead to that the transfer matrices with different spectral parameters commute mutually, i.e., $[t^\circ(u), t^\circ(v)] = 0$. Thus $t^\circ(u)$ is the generating function of conserved quantities and the system is integrable. The Hamiltonian (67) is generated by the transfer matrix $t(u)$ as

$$\begin{aligned} H^\circ &= \eta \left. \frac{\partial \ln t^\circ(u)}{\partial u} \right|_{u=0, \{\theta_j=0\}} - N \\ &= \sum_{n=1}^{N-1} (\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \sigma_n^z \sigma_{n+1}^z) + \frac{\eta}{p} \sigma_1^z + \frac{\eta}{q} (\sigma_N^z + \xi \sigma_N^x). \end{aligned} \quad (67)$$

Following the idea of fusion, we still consider the product of two transfer matrices with certain shift of the spectral parameter

$$\begin{aligned}
 t^o(u)t^o(u-\eta) &= \text{tr}_{1,2} \left\{ K_2^+(u) \mathcal{U}_2(u) K_1^+(u-\eta) \mathcal{U}_1(u-\eta) \right\} \quad \text{[embedded into 2 auxiliary space]} \\
 &= \text{tr}_{1,2} \left\{ K_2^{+t_2}(u) K_1^+(u-\eta) \mathcal{U}_2^{t_2}(u) \mathcal{U}_1(u-\eta) \right\} \\
 &\stackrel{(6)}{=} \frac{1}{\rho_2(2u-\eta)} \text{tr}_{1,2} \left\{ K_2^{+t_2}(u) K_1^+(u-\eta) R_{2,1}^{t_2}(-2u-\eta) R_{1,2}^{t_2}(2u-\eta) \mathcal{U}_2^{t_2}(u) \mathcal{U}_1(u-\eta) \right\} \\
 &= \frac{1}{\rho_2(2u-\eta)} \text{tr}_{1,2} \left\{ (K_1^+(u-\eta) R_{2,1}(-2u-\eta) K_2^+(u)) (\mathcal{U}_2(u) R_{1,2}(2u-\eta) \mathcal{U}_1(u-\eta)) P_{2,1}^{(-)} \right. \\
 &\quad \left. + (K_1^+(u-\eta) R_{2,1}(-2u-\eta) K_2^+(u)) (\mathcal{U}_2(u) R_{1,2}(2u-\eta) \mathcal{U}_1(u-\eta)) P_{2,1}^{(+)} \right\} \\
 &= \Delta^o(u) / \left((u + \frac{\eta}{2})(u - \frac{\eta}{2}) \right) + t_2^o(u), \quad \text{[extract constant factor]} \tag{68}
 \end{aligned}$$

where $\rho_2(u) = -u(u + 2\eta)$.

The first term of Eq.(68) give a number which is the quantum determinant

$$\Delta^{\circ}(u) = a^{\circ}(u)d^{\circ}(u - \eta)(u + \frac{\eta}{2})(u - \frac{\eta}{2}), \quad (69)$$

where the functions $a^{\circ}(u)$ and $d^{\circ}(u)$ are

$$a^{\circ}(u) = \frac{u + \eta}{u + \frac{\eta}{2}}(u + p)(\sqrt{1 + \xi^2}u + q) \prod_{j=1}^N (u - \theta_j + \eta)(u + \theta_j + \eta), \quad (70)$$

$$d^{\circ}(u) = a^{\circ}(-u - \eta) = \frac{u}{u + \frac{\eta}{2}}(u - p + \eta)(\sqrt{1 + \xi^2}(u + \eta) - q) \prod_{j=1}^N (u - \theta_j)(u + \theta_j). \quad (71)$$

The second term of Eq.(68) is a new operator which is the fused transfer matrix up to a constant

$$t_2^{\circ}(u) = \frac{1}{\rho_2(2u - \eta)} \text{tr}_{1,2} \left\{ K_{\{1,2\}}^+(u) T_{\{1,2\}}(u) K_{\{1,2\}}^-(u) \hat{T}_{\{1,2\}}(u) \right\}. \quad (72)$$

From the fusion of the reflection matrices and monodromy matrices

$$\begin{aligned}
 K_{\{1,2\}}^+(u) &= P_{2,1}^{(+)} K_1^+(u - \eta) R_{2,1}(-2u - \eta) K_2^+(u) P_{1,2}^{(+)} = 2u K_{\{1,2\}}^{(1)+}(u), \\
 K_{\{1,2\}}^-(u) &= P_{1,2}^{(+)} K_2^-(u) R_{1,2}(2u - \eta) K_1^-(u - \eta) P_{2,1}^{(+)} = 2u K_{\{1,2\}}^{(1)-}(u), \\
 T_{\{1,2\}}(u) &= P_{1,2}^{(+)} T_2(u) T_1(u - \eta) P_{1,2}^{(+)} = \prod_{l=1}^N (u - \theta_l) T_{\{1,2\}}^{(1, \frac{1}{2})}(u), \\
 \hat{T}_{\{1,2\}}(u) &= P_{2,1}^{(+)} \hat{T}_2(u) \hat{T}_1(u - \eta) P_{2,1}^{(+)} = \prod_{l=1}^N (u + \theta_l) \hat{T}_{\{1,2\}}^{(1, \frac{1}{2})}(u),
 \end{aligned} \tag{73}$$

we obtain

$$t_2^{\circ}(u) = \frac{4u^2}{\rho_2(2u - \eta)} d^{\circ}(u) \mathbb{W}^{\circ}(u), \quad \text{[the constant factor]} \tag{74}$$

where

$$\mathbb{W}^{\circ}(u) = \text{tr}_{\{1,2\}} \left\{ K_{\{1,2\}}^{(1)+}(u) T_{\{1,2\}}^{(1, \frac{1}{2})}(u) K_{\{1,2\}}^{(1)-}(u) \hat{T}_{\{1,2\}}^{(1, \frac{1}{2})}(u) \right\}. \tag{75}$$

Then the operator identity (68) can be expressed as

$$t^\circ(u)t^\circ(u - \eta) = \Delta^\circ(u) \times \text{id}/((u + \frac{\eta}{2})(u - \frac{\eta}{2})) + \frac{4u^2}{\rho_2(2u - \eta)} d^\circ(u)\mathbb{W}^\circ(u). \quad (76)$$

At the inhomogeneous points $\{u = \theta_j\}$, Eq.(76) reduces to

$$(\theta_l + \frac{\eta}{2})(\theta_l - \frac{\eta}{2})t^\circ(\theta_l)t^\circ(\theta_l - \eta) = \Delta^\circ(\theta_l), \quad j = 1, \dots, N. \quad (77)$$

The fusion does not break the integrability of the system, thus the transfer matrix and the fused transfer matrix commute with each other. Thus they have common eigenstates. Acting the operator relation (76) on a common eigenstate, we obtain the $t - W$ relation

$$\Delta^\circ(u) - (u + \frac{\eta}{2})(u - \frac{\eta}{2})\bar{\Lambda}(u)\bar{\Lambda}(u - \eta) = u^2 \prod_{j=1}^N (u - \theta_j)(u + \theta_j) \bar{W}(u), \quad (78)$$

where $\bar{\Lambda}(u)$ and $\bar{W}(u)$ are the eigenvalues of the transfer matrix $t^\circ(u)$ and the fused one $\mathbb{W}^\circ(u)$, respectively. At the points of inhomogeneous point, the eigenvalue $\bar{\Lambda}(u)$ satisfies

$$(\theta_l + \frac{\eta}{2})(\theta_l - \frac{\eta}{2})\bar{\Lambda}(\theta_l)\bar{\Lambda}(\theta_l - \eta) = \Delta^\circ(\theta_l), \quad j = 1, \dots, N. \quad (79)$$

Exact solution

II. Heisenberg spin chains without $U(1)$ -symmetry: nondiagonal boundary condition

The exact solution of the system does not depend on the inhomogeneous parameters. Thus we set them as zero. From the definitions, we know that the eigenvalue function $\bar{\Lambda}(u)$ is a polynomial of u with degree $2N + 2$ and also satisfies the crossing symmetry and asymptotic behavior

$$\bar{\Lambda}(-u - \eta) = \bar{\Lambda}(u), \quad \lim_{u \rightarrow \infty} \bar{\Lambda}(u) = 2u^{2N+2} + \dots \quad (80)$$

The eigenvalue function $\bar{W}(u)$ is an polynomial of u with degree of $2N + 4$ and has asymptotic behavior

$$\bar{W}(-u) = \bar{W}(u), \quad \lim_{u \rightarrow \infty} \bar{W}(u) = (\xi^2 - 3)u^{2N+4} + \dots \quad (81)$$

Based on above analysis, we parameterized $\bar{\Lambda}(u)$ and $\bar{W}(u)$ as

$$\bar{\Lambda}(u) = 2 \prod_{j=1}^{N+1} \left(u - z_j + \frac{\eta}{2}\right) \left(u + z_j + \frac{\eta}{2}\right), \quad (82)$$

$$\bar{W}(u) = (\xi^2 - 3) \prod_{k=1}^{N+2} (u - w_k)(u + w_k), \quad (83)$$

where $\{z_j | j = 1, \dots, N + 1\}$ and $\{w_k | k = 1, \dots, N + 2\}$ are the roots of corresponding polynomials,

which are completely determined by the BAEs

$$\Delta(z_j - \frac{\eta}{2}) = (z_j - \frac{\eta}{2})^{2N+2} \bar{W}(z_j - \frac{\eta}{2}), \quad j = 1, \dots, N+1, \quad (84)$$

$$\Delta(w_k) = (w_k + \frac{\eta}{2})(w_k - \frac{\eta}{2}) \bar{\Lambda}(w_k) \bar{\Lambda}(w_k - \eta), \quad k = 1, \dots, N+2, \quad (85)$$

where $\Delta(u)$ is the quantum determinant with homogeneous limit $\{\theta_j = 0\}$

$$\Delta(u) = (u - \eta)(u + \eta)(u - p)(u + p)(\sqrt{1 + \xi^2} u + q)(\sqrt{1 + \xi^2} u - q)(u + \eta)^{2N}(u - \eta)^{2N}. \quad (86)$$

The eigenvalue of the Hamiltonian (67) is determined by the solutions of above BAEs

$$E^o = \sum_{j=1}^{N+1} \frac{\eta^2}{\frac{\eta^2}{4} - z_j^2} - N. \quad (87)$$

Structure of roots

II. Heisenberg spin chains without $U(1)$ -symmetry: nondiagonal boundary condition

The hermitian of Hamiltonian (67) requires that the boundary parameters satisfy

$$p^* = -p, \quad q^* = -q, \quad \xi^* = \xi. \quad (88)$$

The above constrains implies

$$R^\dagger(u) = -R(-u^*), \quad \left(K^{(\pm)}(u)\right)^\dagger = -K^{(\pm)}(-u^*), \quad (89)$$

which gives rise to the hermitian properties of the transfer matrix and its eigenvalue

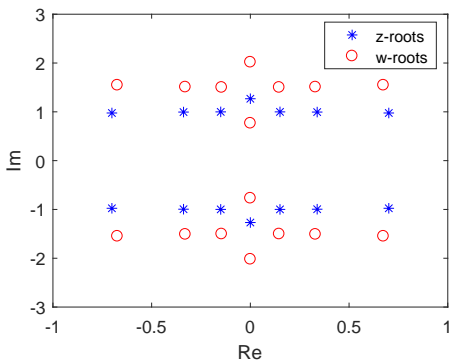
$$\left(t^\circ(u)\right)^\dagger = t^\circ(-u^*), \quad \bar{\Lambda}^*(u) = \bar{\Lambda}(-u^*). \quad (90)$$

Combining the expansions (82) and (83), $t - W$ relation (78) and the hermitian relation (90), we conclude that if z_j is a root of $\bar{\Lambda}(u)$, then z_j^* must be the root and that if w_j is a root of $\bar{W}(u)$, then w_j^* must be the root, which can be denoted as

$$\{z_j^*\} = \{z_j\}, \quad \{w_j^*\} = \{w_j\}. \quad (91)$$

Structure of roots

II. Heisenberg spin chains without $U(1)$ -symmetry: nondiagonal boundary condition



The patterns of z -roots (blue asterisks) and w -roots (red circles) in complex plane at the ground state with $N = 6, \eta = i, \rho = -1.2i, \bar{q} = 0.8i, \xi = 1, \{\theta_j = 0\}$.

- The zero roots form the conjugate pairs around the line $\pm \frac{l\eta}{2}$ with a positive integer $l \geq 2$, which is called as the l -strings.
- At the ground state, both z -roots and w -roots form the 2-strings with $l = 2, 3$ respectively.
- **Boundary strings:** Boundary conjugate pairs at the imaginary axis.

Ground state eigenfunctions in the thermodynamic limit

II. Heisenberg spin chains without $U(1)$ -symmetry: nondiagonal boundary condition

Parameterization for the ground state:

- Denote the z -roots as $\{\pm z_1 \eta, u_j^{(2)} \pm \eta | j = 1, \dots, N\}$, with $z_1, u_j^{(2)} \in \mathfrak{R}$.
- Denote the w -roots as $\{\pm \chi_1 \eta, \pm \chi_2 \eta, w_j^{(2)} \pm \frac{3\eta}{2} | j = 1, \dots, N\}$, with $\chi_1, \chi_2, w_j^{(2)} \in \mathfrak{R}$.

Substituting these 2-strings into Eqs.(82) and (83), we obtain

$$\begin{aligned}\bar{\Lambda}_g(u) &= 2(u - (z_1 - \frac{1}{2})\eta)(u + (z_1 + \frac{1}{2})\eta) \prod_{j=1}^{N/2} (u - u_j^{(2)} - \frac{\eta}{2})(u + u_j^{(2)} - \frac{\eta}{2}) \\ &\quad \times (u - u_j^{(2)} + \frac{3\eta}{2})(u + u_j^{(2)} + \frac{3\eta}{2}) \\ &= 2(u - (z_1 - \frac{1}{2})\eta)(u + (z_1 + \frac{1}{2})\eta) e^{2N(\bar{\lambda}_g^{(0)}(u) + \frac{1}{2N}\bar{\lambda}_g^{(1)}(u) + O(\frac{1}{N^2}))},\end{aligned}\quad (92)$$

$$\bar{\Lambda}_g(0) = 2(z_1 - \frac{1}{2})(z_1 + \frac{1}{2}) e^{2N(\bar{\lambda}_g^{(0)}(u) + \frac{1}{2N}\bar{\lambda}_g^{(1)}(u) + O(\frac{1}{N^2}))} = 2pq \equiv 2p\bar{q}\sqrt{1 + \xi^2}.\quad (93)$$

Ground state eigenfunctions in the thermodynamic limit

II. Heisenberg spin chains without $U(1)$ -symmetry: nondiagonal boundary condition

$$\begin{aligned}\bar{W}_g(u) &= (\xi^2 - 3)(u - \chi_1\eta)(u + \chi_1\eta)(u - \chi_2\eta)(u + \chi_2\eta) \\ &\quad \times \prod_{j=1}^{N/2} (u - w_j^{(2)} - \frac{3}{2}\eta)(u + w_j^{(2)} - \frac{3}{2}\eta)(u - w_j^{(2)} + \frac{3}{2}\eta)(u + w_j^{(2)} + \frac{3}{2}\eta) \\ &= (\xi^2 - 3)(u - \chi_1\eta)(u + \chi_1\eta)(u - \chi_2\eta)(u + \chi_2\eta)e^{2N(\bar{\omega}_g^{(0)}(u) + \frac{1}{2N}\bar{\omega}_g^{(1)}(u) + O(\frac{1}{N^2}))},\end{aligned}\quad (94)$$

where the leading terms are determined by

$$\frac{\partial}{\partial u} \bar{\lambda}_g^{(\beta)}(u) = \int_{-\infty}^{\infty} \left(\frac{1}{u - \lambda - \frac{\eta}{2}} + \frac{1}{u - \lambda + \frac{3\eta}{2}} \right) \rho_g^{(\beta)}(\lambda) d\lambda, \quad \beta = 0, 1, \quad (95)$$

$$\frac{\partial}{\partial u} \bar{\omega}_g^{(\beta)}(u) = \int_{-\infty}^{\infty} \left(\frac{1}{u - \lambda - \eta} + \frac{1}{u - \lambda + \eta} + \frac{1}{u - \lambda - 2\eta} + \frac{1}{u - \lambda + 2\eta} \right) \rho_w^{(\beta)}(\lambda) d\lambda. \quad (96)$$

Ground state eigenfunctions in the thermodynamic limit

II. Heisenberg spin chains without $U(1)$ -symmetry: nondiagonal boundary condition

Taking the difference of (79) at two inhomogeneous points and considering the continuum limit, we have

$$\frac{\partial}{\partial u} \ln \left[\left(u + \frac{\eta}{2} \right) \left(u - \frac{\eta}{2} \right) \bar{\lambda}(u) \bar{\lambda}(u - \eta) \right] = \frac{\partial}{\partial u} \ln \Delta(u) + O\left(\frac{1}{N}\right). \quad (97)$$

Similarly with the periodic boundary case, substituting (92) into (97), we have

$$\begin{aligned} \frac{\partial}{\partial u} [\bar{\lambda}_g^{(0)}(u) + \bar{\lambda}_g^{(0)}(u - \eta)] &= \frac{1}{u + \eta} + \frac{1}{u - \eta}, \quad \bar{\lambda}_g^{(0)}(0) = 0, \\ \frac{\partial}{\partial u} [\bar{\lambda}_g^{(1)}(u) + \bar{\lambda}_g^{(1)}(u - \eta)] &= \frac{1}{u + \eta} + \frac{1}{u - \eta} + \frac{1}{u + p\eta} + \frac{1}{u - p\eta} + \frac{1}{u + \bar{q}\eta} + \frac{1}{u - \bar{q}\eta} \\ &\quad - \frac{1}{u + \frac{\eta}{2}} - \frac{1}{u - \frac{\eta}{2}} - \frac{1}{u + \frac{\eta}{2}} - \frac{1}{u - \frac{\eta}{2}} - \frac{1}{u + (z_1 - \frac{1}{2})\eta} - \frac{1}{u - (z_1 - \frac{1}{2})\eta} \\ &\quad - \frac{1}{u + (z_1 + \frac{1}{2})\eta} - \frac{1}{u - (z_1 + \frac{1}{2})\eta}, \\ \bar{\lambda}_g^{(1)}(0) &= \ln(2p\bar{q}\sqrt{1 + \xi^2}) - \ln \left[2(z_1 + \frac{1}{2})(z_1 - \frac{1}{2}) \right]. \end{aligned} \quad (98)$$

Ground state eigenfunctions in the thermodynamic limit

II. Heisenberg spin chains without $U(1)$ -symmetry: nondiagonal boundary condition

Substituting (95) into (98) and solving it by the Fourier transformation, we obtain the densities of z -roots at the ground state as

$$\begin{aligned}\tilde{\rho}_g^{(0)}(w) &= \frac{a_2(w)}{2\pi[a_1(w) + a_3(w)]}, \\ \tilde{\rho}_g^{(1)}(w) &= \frac{1}{2\pi[a_1(w) + a_3(w)]} [a_2(w) + a_{2p}(w) + a_{2\bar{q}}(w) - a_1(w) - a_{2z_1-1}(w) - a_{2z_1+1}(w)],\end{aligned}\quad (99)$$

where $\tilde{\rho}_g^{(\beta)}(w)$ is the Fourier transformation of $\rho_g^{(\beta)}(\lambda)$ and $a_n(w) = e^{-n|w|/2}$. By incorporating the 2-string structure into the energy expression (87) and integrating it with the densities (99) as the weighting factor, we obtain the ground state energy

$$\begin{aligned}E_g^o &= -Ni \int_{-\infty}^{\infty} \left(\frac{1}{z + \frac{i}{2}} + \frac{1}{z - \frac{3i}{2}} \right) \int_{-\infty}^{\infty} e^{i\omega z} (\tilde{\rho}_g^{(0)}(w) + \tilde{\rho}_g^{(1)}(w)) d\omega dz + \frac{1}{z_1^2 - \frac{1}{4}} - N \\ &= (1 - 4 \ln 2)N - 1 + \pi - 2 \ln 2 + \frac{1}{|p|} + \frac{\sqrt{1 + \xi^2}}{|q|} - 2i \int_0^{\infty} \frac{e^{-|p|w} + e^{-\frac{|q|w}{\sqrt{1+\xi^2}}}}{1 + e^{-w}}.\end{aligned}\quad (100)$$

Ground state eigenfunctions in the thermodynamic limit

II. Heisenberg spin chains without $U(1)$ -symmetry: nondiagonal boundary condition

Substituting the densities (99) into (95), we arrive at

$$\bar{\lambda}_g^{(0)}(u) = \ln \frac{2\Gamma(1 + \frac{i u}{2})\Gamma(\frac{3}{2} - \frac{i u}{2})}{\Gamma(\frac{1}{2} + \frac{i u}{2})\Gamma(1 - \frac{i u}{2})}, \quad (101)$$

$$\begin{aligned} \bar{\lambda}_g^{(1)}(u) = & \ln \left[\frac{4\sqrt{1 + \xi^2}}{(u - (z_1 - \frac{1}{2})\eta)(u + (z_1 + \frac{1}{2})\eta)(u + \frac{\eta}{2})} \frac{\cosh(\frac{\pi u}{2} - \frac{i\pi}{4})}{\sinh(\frac{\pi u}{2} - \frac{i\pi}{4})} \frac{\Gamma(1 + \frac{i u}{2})\Gamma(\frac{3}{2} - \frac{i u}{2})}{\Gamma(\frac{1}{2} + \frac{i u}{2})\Gamma(1 - \frac{i u}{2})} \right. \\ & \left. \times \frac{\Gamma(\frac{p+1}{2} + \frac{i u}{2})\Gamma(\frac{p+2}{2} - \frac{i u}{2})}{\Gamma(\frac{p}{2} + \frac{i u}{2})\Gamma(\frac{p+1}{2} - \frac{i u}{2})} \frac{\Gamma(\frac{\bar{q}+1}{2} + \frac{i u}{2})\Gamma(\frac{\bar{q}+2}{2} - \frac{i u}{2})}{\Gamma(\frac{\bar{q}}{2} + \frac{i u}{2})\Gamma(\frac{\bar{q}+1}{2} - \frac{i u}{2})} \right], \quad (102) \end{aligned}$$

which implies

$$\begin{aligned} \bar{\lambda}_g(u) = & \frac{8\sqrt{1 + \xi^2}}{u + \frac{\eta}{2}} \frac{\cosh(\frac{\pi u}{2} - \frac{i\pi}{4})}{\sinh(\frac{\pi u}{2} - \frac{i\pi}{4})} \frac{\Gamma(1 + \frac{i u}{2})\Gamma(\frac{3}{2} - \frac{i u}{2})}{\Gamma(\frac{1}{2} + \frac{i u}{2})\Gamma(1 - \frac{i u}{2})} \frac{\Gamma(\frac{p+1}{2} + \frac{i u}{2})\Gamma(\frac{p+2}{2} - \frac{i u}{2})}{\Gamma(\frac{p}{2} + \frac{i u}{2})\Gamma(\frac{p+1}{2} - \frac{i u}{2})} \\ & \times \frac{\Gamma(\frac{\bar{q}+1}{2} + \frac{i u}{2})\Gamma(\frac{\bar{q}+2}{2} - \frac{i u}{2})}{\Gamma(\frac{\bar{q}}{2} + \frac{i u}{2})\Gamma(\frac{\bar{q}+1}{2} - \frac{i u}{2})} \left(\frac{2\Gamma(1 + \frac{i u}{2})\Gamma(\frac{3}{2} - \frac{i u}{2})}{\Gamma(\frac{1}{2} + \frac{i u}{2})\Gamma(1 - \frac{i u}{2})} \right)^{2N} e^{O(\frac{1}{N})}. \quad (103) \end{aligned}$$

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Now, we consider the leading terms of the $\bar{W}_g(u)$ in the thermodynamic limit. Analogous to the case of periodic boundary condition, we set the variable $z_j = u_j^{(2)} + \eta$ in BAEs (84) and multiply it by its conjugate counterpart. As a result, we obtain

$$\Delta(u_j^{(2)} + \frac{\eta}{2})\Delta(u_j^{(2)} - \frac{\eta}{2}) = (u_j^{(2)} + \frac{\eta}{2})^{2N+2}(u_j^{(2)} - \frac{\eta}{2})^{2N+2} \bar{W}(u_j^{(2)} + \frac{\eta}{2})\bar{W}(u_j^{(2)} - \frac{\eta}{2}). \quad (104)$$

By taking the derivative of the logarithm of (104), we obtain

$$\begin{aligned} \frac{1}{2N} \frac{\partial}{\partial u} \ln[W(u + \frac{\eta}{2})W(u - \frac{\eta}{2})] &= \frac{1}{2N} \frac{\partial}{\partial u} \left(\ln [\Delta(u + \frac{\eta}{2})\Delta(u - \frac{\eta}{2})] \right. \\ &\quad \left. - \ln [(u + \frac{\eta}{2})^{2N+2}(u - \frac{\eta}{2})^{2N+2}] \right) + O\left(\frac{1}{N^2}\right). \end{aligned} \quad (105)$$

Substituting (94) and (96) into (105), and solving it by the Fourier transformation, we have the densities

$$\tilde{\rho}_w^{(0)}(w) = \frac{a_2(w)}{2\pi[a_1(w) + a_3(w)]}, \quad (106)$$

$$\begin{aligned} \tilde{\rho}_w^{(1)}(w) &= \frac{1}{2\pi[a_1(w) + a_3(w)]} [a_3(w) + a_{2p+1}(w) + a_{2p-1}(w) + a_{2\bar{q}+1}(w) + a_{2\bar{q}-1}(w) \\ &\quad - a_1(w) - a_{2\chi_1-1}(w) - a_{2\chi_1+1}(w) - a_{2\chi_2-1}(w) - a_{2\chi_2+1}(w)]. \end{aligned} \quad (107)$$

Ground state eigenfunctions in the thermodynamic limit

II. Heisenberg spin chains without $U(1)$ -symmetry: nondiagonal boundary condition

Substituting the densities (106) and (107) into (96), we arrive at

$$\frac{\partial}{\partial u} \bar{\omega}_g^{(0)}(u) = \frac{\partial}{\partial u} \ln \frac{\Gamma(\frac{3}{2} + \frac{i u}{2}) \Gamma(\frac{3}{2} - \frac{i u}{2})}{\Gamma(1 + \frac{i u}{2}) \Gamma(1 - \frac{i u}{2})} = \frac{\partial}{\partial u} \ln \left[\frac{(u + \eta)(u - \eta)}{2u} \tanh \frac{\pi u}{2} \right], \quad (108)$$

$$\begin{aligned} \frac{\partial}{\partial u} \bar{\omega}_g^{(1)}(u) &= \frac{\partial}{\partial u} \ln \left(\frac{(u - p\eta)(u + p\eta)(u - \bar{q}\eta)(u + \bar{q}\eta)}{(u - \chi_1\eta)(u + \chi_1\eta)(u - \chi_2\eta)(u + \chi_2\eta)} \frac{\Gamma(\frac{3}{2} + \frac{i u}{2}) \Gamma(\frac{3}{2} - \frac{i u}{2})}{\Gamma(1 + \frac{i u}{2}) \Gamma(1 - \frac{i u}{2})} \right. \\ &\quad \left. \times \frac{\Gamma(\frac{1}{2} + \frac{i u}{2}) \Gamma(\frac{1}{2} - \frac{i u}{2})}{\Gamma(1 + \frac{i u}{2}) \Gamma(1 - \frac{i u}{2})} \right). \end{aligned} \quad (109)$$

Then the leading terms can be obtained by taking the integration of above equation and the final results are

$$\bar{\omega}_g^{(0)}(u) = \ln \left(\frac{\bar{C}_w^{(0)}}{2} \frac{(u + \eta)(u - \eta)}{u} \tanh \frac{\pi u}{2} \right), \quad (110)$$

$$\begin{aligned} \bar{\omega}_g^{(1)}(u) &= \ln \left(\frac{(u - p\eta)(u + p\eta)(u - \bar{q}\eta)(u + \bar{q}\eta)}{(u - \chi_1\eta)(u + \chi_1\eta)(u - \chi_2\eta)(u + \chi_2\eta)} \frac{\Gamma(\frac{3}{2} + \frac{i u}{2}) \Gamma(\frac{3}{2} - \frac{i u}{2})}{\Gamma(1 + \frac{i u}{2}) \Gamma(1 - \frac{i u}{2})} \frac{\Gamma(\frac{1}{2} + \frac{i u}{2}) \Gamma(\frac{1}{2} - \frac{i u}{2})}{\Gamma(1 + \frac{i u}{2}) \Gamma(1 - \frac{i u}{2})} \right) \\ &\quad + \ln \bar{C}_w^{(1)}. \end{aligned} \quad (111)$$

Ground state eigenfunctions in the thermodynamic limit

II. Heisenberg spin chains without $U(1)$ -symmetry: nondiagonal boundary condition

Thus the the ground state eigenfunction $\bar{W}_g(u)$ in the thermodynamic limit can be expressed as

$$\begin{aligned}\bar{W}_g(u) &= 4\bar{C}_w^{(1)}(\xi^2 - 3)(u - p\eta)(u + p\eta)(u - \bar{q}\eta)(u + \bar{q}\eta) \tanh^2 \frac{\pi u}{2} \\ &\quad \times \frac{(u + \eta)^{2N+1}(u - \eta)^{2N+1}}{u^{2N+2}} \left(\frac{\bar{C}_w^{(0)}}{2} \tanh \frac{\pi u}{2} \right)^{2N}.\end{aligned}\quad (112)$$

Substituting Eq.(112) into the $t - W$ relation (78), we have

$$\begin{aligned}\left(u + \frac{\eta}{2}\right)\left(u - \frac{\eta}{2}\right)\bar{\Lambda}_g(u)\bar{\Lambda}_g(u - \eta) &= (1 + \xi^2)(u - p\eta)(u + p\eta)(u - \bar{q}\eta)(u + \bar{q}\eta) \\ &\quad \times (u - \eta)^{2N+1}(u + \eta)^{2N+1} \left\{ 1 - \frac{4(\xi^2 - 3)}{1 + \xi^2} \bar{C}_w^{(1)} \tanh^2 \frac{\pi u}{2} \left(\frac{\bar{C}_w^{(0)}}{2} \tanh \frac{\pi u}{2} \right)^{2N} e^{O(\frac{1}{N})} \right\}.\end{aligned}\quad (113)$$

When u tends to infinity, the coefficient of the highest order term of the left hand side of (113) is 4. Thus the corresponding coefficient of the right hand side of (113) should be also 4, which gives $\bar{C}_w^{(0)} = 2$ and $\bar{C}_w^{(1)} = \frac{1}{4}$. Because $\tanh \frac{\pi u}{2} < 1$, the second term of the right hand side of (113) is negligible in the thermodynamic limit.

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- The **exact solutions** of the model with periodic and generic open boundary conditions.
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- Serves as a compelling **proof** of the validity of the extensively applied inversion relation.

Thanks for your attention